Calcite Palaeopiezometry

Laboratory notes

Kamil Kosiorek

9650958

Supervised by Ernest Rutter and Steve Covey-Crump

This document is composed of two parts:

Part 1: Progress log – Organisational notes, progress updates, planning.

Part 2: Handwritten laboratory notes – complete record of though development and workings.

All entries are dated, and no entries were edited or removed.

Calcite Palaeopiezometry
Progress log

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Instructions:

Date all the entries, do not edit or delete past entries. When adding comments, date them. Name the relevant files and their locations.

29th October 2020

Edit by Kamil on 30/10/2020:

Only just started looking into the project. I had a meeting with Ernest sometime in June, but I forgot most of what was said. I remember struggling with understanding what the project is about exactly. Ernie sent me some papers to read, but I found them somewhat challenging. I have all the data.

I have decided to:

- Learn a bit more about crystallography. Firstly, by reading the Earth Materials textbook by Klein and Philpotts.
- Learn a bit more about calcite
- Read papers listed by Ernie
- Find more relevant literature

So far, I have read chapter 4 of Klein and Philpotts, and understand (I think) the Miller indices. This is a bit more complex for the 4-axis hexagonal system that calcite is a part of.

I have started a 'lab-book' – just a notebook with all the raw notes I collect.

30th October 2020

Edit by Kamil on 30/10/2020:

Continued reading of the Klein and Philpotts textbook – I learned about the 4-axis hexagonal Miller indices, and about how the stereonet projection works for hexagonal crystal systems. Identified calcite as $\bar{3}\ 2/m$ in the Hermann-Mauguin notation.

Learned a bit about how stereonets for hexagonal systems work. Saw examples of rhombohedron and hexagonal scalenohedron - though I'm not sure which 'form' I should care about for the analysis – or perhaps there is more? The symmetry is the same, but stereonets look different (face projections).

31st October 2020

Edit by Kamil on 31/10/2020:

Understood what chirality means for scalenohedron form, and how stereoplots are projected from upper hemisphere – also how crystal axes always go through the edges of the crystal.

Got myself a few rhombohedral calcite blocks to help with visualisation.

3rd December 2020

Edit by Kamil on 05/12/2020:

I had a zoom meeting with Steve. I explained where I am standing, and explained how the more I read, the less I feel know. We spoke about some of the experiment details, and about some of the geometry. Steve helped me paint the bigger picture.

Steve suggested that work & reading should go in pair, and that I should try to analyse the data as I get to it – without necessarily fully understanding the next step or having a complete image of the bigger picture. I think he might be right.

Steve suggested I set up a zoom meeting with Ernie. I am trying to get that arranged for sometime in the next 2 weeks.

22nd December 2020

Edit by Kamil on 04/03/2021:

Had a zoom meeting with Ernie. We discussed (fill)

4th March 2021

Edit by Kamil on 04/03/2021:

Last week I submitted an assignment for a different module which focused on EBSD, a technique used to tell the orientation of grains. I feel like I understand it well now.

Today I re-watched Ernie's first lecture and made some better notes on orientation presentation, Turner method, and yield stress criteria/analysis.

5th March 2021

Edit by Kamil on 08/03/2021:

I re-watched Ernie's second lecture and made more notes on topics touched.

8th March 2021

Edit by Kamil on 08/03/2021:

I made some detailed notes on EBSD – however there is an even better account of the EBSD technique in the piece of work I wrote for Analytical Techniques 2 weeks ago.

9th - 15th March 2021

Edit by Kamil on 15/03/2021:

Over the past days I have re-read the relevant literature and took notes. I feel like I know how to tackle the data, however I am still not 100% clear on the exact parameters used during the experiment. I need to work on that next.

23rd March 2021

Edit by Kamil on 23/03/2021:

Got an email from Ernie outlining the 'disciplinary' plan for getting the project done. To be honest this is quite useful, as I am lost in the maths and the order things come in. He has provided solutions for quite a few of the grains – this may be good framework for what I'm meant to do. And then to somehow link it to the stress. I need to read his description on a soon basis.

We agreed that I will produce preliminary background + intro sections for April 6th.

24th March 2021

Edit by Kamil on 24/03/2021:

Yesterday I asked Ernie some of the questions I had written down. They're regarding stress homogeneity, finding e+a/h fabric in natural rocks, and re-crystallisation. Ernie provided answers, with reference to the Spiers 1980 paper. Steve 'translated' the bit on stress homogeneity and how I can apply it to my project – either I observe it and it's relevant, or I don't and it's part of background.

26th March 2021

Edit by Kamil on 26/03/2021:

I read the document on stress and strain. I was hoping to also read the Spiers paper and make notes on both, but ran out of time.

27th March 2021

Edit by Kamil on 28/03/2021:

I covered 20 pages of the Pet Engineering document, and still need to look at a few sections of (Intracrystalline plasticity) etc.

5th April 2021

Edit by Kamil on 05/04/2021:

Took a few day long break for Easter and to complete other coursework. Yesterday I finished the engineering document, and today I had a look at the detailed work-through of the Calcite data that Ernie sent me as aid. I also read the Spiers 1980 paper which addresses the stress homogeneity and strain heterogeneity in deformed samples – and Ernie actually touched on how cross-sectional estimation of stress may be a bit too simplistic. I'll need to look at it later.

I looked into running MTEX on my Matlab, but with no result. I am getting an error when trying to input data. I updated my Matlab but still get the same error.

I think I will have to do without MTEX – perhaps with just other stereonet plotting software and drawing package touch-ups like Ernie suggested.

7th April 2021

Edit by Kamil on 07/04/2021:

Yesterday I worked on the Euler angle problems – still figuring out which way is up.

Today I finally created the dissertation word file. I made an outline of what goes in each section, but this will need to be updated with details from correspondence with Ernie – I've already noticed it answers some questions I had, but won't have the time to do it today.

11th April 2021

Edit by Kamil on 12/04/2021:

I have looked into the spherical approximation for stress that Ernie spoke about – it is simple enough to apply mathematically. I was initially worried that I would have to struggle with grains located off-axis, but Ernie re-assured me that because of the geometry and scale of the section, it is okay to assume all grains are effectively on-axis.

12th April 2021

Edit by Kamil on 12/04/2021:

Today I looked into the Bunge convention and all the files provided by Dave Wallis. I noticed that we can't seem to agree on what Bunge really means – I think all angles should be right-handed (anticlockwise), but the manual for the CHANNEL software defines E1 and E3 as opposite sense to E2. Some other source I found on the internet lists them all as right-handed. I asked Ernie for input.

13th April 2021

Edit by Kamil on 13/04/2021:

In the morning I figured out the Bunge conventions. Does not actually matter how I take them, as sample is axi-symmetric. In the worst case scenario, I'll have a reflection of what Ernie worked on, but both are equally valid. In fact, the stereonet plot I produced is rotated by 90 degrees anticlockwise compared to Ernie's.

In the evening I figured out the spherical cap correction for stress trajectories/isobars. It was actually quite a pleasant day of coding.

14th April 2021

Edit by Kamil on 14/04/2021:

I extracted the stress profile of my sample, and matched the grains to it, so now I know the approximate stress that each grain experienced. I also made some diagrams which may be useful for the dissertation itself.

I noticed that the assumption about strain being largely irrelevant for sample geometry may not be strictly true, as even though the strain is ~1%, it's not homogenous. The central part is more strained. I did ask Ernie if I should account for this, but apparently this sort of correction is minor compared to uncertainties introduced by stress heterogeneities due to the grains themselves.

I also had a read of the document guidelines. I need to adjust my font and font size, but also look at the 'figure list' section.

15th April 2021

Edit by Kamil on 15/04/2021:

I started preparing the channelling-montage and the band-contrast images for the twin trace extraction exercise – I made both images into one long record and I labelled the grains. Some are problematic, as I discovered the two images do not exactly match. I asked Ernie why. I think it is to do with the geometry at which they were collected – but that still does not explain why some small grains are present on one image and not the other and vice versa.

I wanted to index the images with sample dimensions in matlab today, but my computer decided to force a loooong windows update, so that's a task for tomorrow.

20th April 2021

Edit by Kamil on 20/04/2021:

Today I plotted the twin c-axes onto the stereonets and found a way to connect them with arcs. I verified the host c-axis to twin c-axis angle, which should be 52°, and in most cases is. Grain 26 shows an angle of 83.85°, which like Ernie suggested, is probably an anomaly in the measurement.

The goal for tomorrow is to figure out how to get the rotation towards the sigma 1. I'm thinking of doing a rotation matrix, but I think it will be a bit of trial and error.

21st April 2021

Edit by Kamil on 21/04/2021:

I found something called "Rodrigues' rotation formula". It allows for easy rotation of a unit vector around a specified axis. Very useful for going to the e-plane by going from 26 degrees from c-axis first (towards m-axis), and then going 60 degrees around the original c-axis so that I index with the c-e plane mirror axis, not the r-plane containing part of it.

I wrote two matlab functions – one that extracts cosines from Euler, and another that carries out the Rodrigues' rotations. I tested them on a few data points to see if I can get from host orientation alone to the measured twin. I can. One of the three solutions will be within 2° and others are about 85° away. I find that the solution tends to be the one at 240° index, except when two twins are present – then it is common that solution is at 180°, not 2°, away – this is a symmetry consideration for later.

22nd April 2021

Edit by Kamil on 22/04/2021:

In the morning I confirmed that once the hosts are rotated so that c-axis is coincident with the twin's (as measured by EBSD), the remaining axes can also by aligned by either 0, 1, or 2 rotations by 120°.

I wrote some code that travels a specified number of degrees from the c-axis towards the c-e plane, and then rotates 120 degrees twice, giving me orientations of all possible twin c-axes (but not all twin axes, as there are still three possibilities for each of 3 axes – this isn't exactly relevant because of symmetry though). Aim is to use this later to simulate the three possibilities and choose the best one based on the image – i.e. align twin traces. I will also need to do the same for the r-planes, which should be an easy adaptation of the same code.

Next, I wrote a piece of code that allows me to translate any vector expressed as direction cosines into plunge/azimuth format, so I can plot it on my stereonets. I checked the results against plotting directly from Euler, and method seems to work fine.

Because I wrote so many matlab functions by now, I made a word file which summarises the library of code I created – this will aid me in finding the right function when I need it.

Edit by Kamil on 22/04/2021, late evening:

I worked out how to index and find the right solution for the EBSD measured twins – and how I can then go 72 degrees (26+45) from c-axis in that direction along c-e plane to find the sigma 1 direction – I plotted those on the stereonet. They make sense. Grain 26 is removed from analysis, and so may be grain 135 – it indexes 10 degrees away from measured twin. Most other grains do so within 2 degrees. The 10 degrees are quite noticeable on the stereonet.

23rd April 2021

Edit by Kamil on 23/04/2021:

I worked out sigma 3. Then I plotted it on the stereonets and did contours. It shows roughly what I expected. Spread out around a great circle perpendicular to sigma 1, albeit also slightly tilted. Ernie thinks this tilt of ~20° may be significant and suggested it's due to pre-existing fabric. I think it may be because the sample was mis-aligned on the EBSD stage. It's something I need to keep in mind.

While sigma 3 is at -19° to c-axis, I used the value of -18.9° to avoid ambiguity with plotting arcs between sigma 1 and sigma 3 on the stereonet – as I always choose the acute angle.

I also tidied up the textfile tables – I wrote a piece of code that helps with their formatting, so they should be more readable.

I also devised a method for getting the potential trace of the e-plane out of the host orientation, but I have not yet had the time to implement it.

27th April 2021

Edit by Kamil on 27/04/2021:

I plotted the second twin sigma 1, sigma 3, and twin c-axis. It works fine, but I need to think about the implications of the 109.94° separation between the two predicted sigma 1 directions. This is expected – but what I need to consider for the Schmid factor analysis later, is that on top of the angle in the c-e plane, I need to consider the angle that the sigma 1 vector makes with the c-e plane, as that's where the slip vector is – something to think about.

I used the Miller-Bravais indices to confirm the angular relationships in calcite. That is, the 26° between c-axis and e-pole, 44° between c-axis and r-pole, and 63° between the c-axis and f-pole.

28th April 2021

Edit by Kamil on 28/04/2021:

I worked out the e-poles, r-poles, and their corresponding traces on the image plane. Doing the cross product of e-pole with [0,0,1] – the image z-axis, did work fine to produce traces.

I tested this with Euler angles of zero – results are as expected. I then tested it against a few grains with known twin orientations. Both methods produce the same solution index, so I will be able to find the correct of the three solutions for each twinned grain.

I made some corrections – previously images were squished, sometimes showing small angle discrepancies. Now this should not happen.

I changed the approach to collecting traces as well – instead of plotting the trace figures on top of the image using grain coordinates, I instead generated 'expected traces' figure for each grain, and will overlay this on top of the channelling image in Illustrator – this approach is more manual, but gives me more freedom in moving the axes around the image, which will allows me to better judge the angles.

After plotting a few grains and seeing planes that I don't expect to see, I decided that I will include the f-slip system as well – just to see if it helps to determine what is and what is not an e-plane.

29th April 2021

Edit by Kamil on 29/04/2021:

Went through the first 164 grains, with 159 left for tomorrow (hopefully). I made a list of all the grains that have problems with them. So far, the 'problem' list includes 54 grains (33% of all analysed). Some of the problems are minor, such as small angle discrepancies, or inability to see small grains properly (they likely are untwined). Bigger problem is the ambiguity when one or two of the potential solutions align with themselves, or with one of the f or r planes.

I found that e-planes from smaller grains seem to propagate through bigger grains. Sometimes even through entire image. Perhaps this is because the energy required to twin a small grain is enough to fracture the surrounding grains too? Or perhaps those lines are just artifacts.

30th April 2021

Edit by Kamil on 30/04/2021:

Gathered twin solutions for the remaining grains. 108 of the 323 are 'problematic'. Roughly 1/3rd. That's still quite an improvement. In total there is

341 twin planes now, but this includes the problematic ones too. I will have the number of good twins soon.

1st May 2021

Edit by Kamil on 01/05/2021:

Generated all the twins and picked out only the solutions that I observed. Then I developed code that translates direction cosines back into Euler angles, as this will be easier to feed into the code that already exists. I double checked it all translates back into the cosines the way I want to – it does.

I sent Ernie all the twinned grains I gathered – 216 of which are non-problematic.

2nd May 2021

Edit by Kamil on 02/05/2021:

Wrote code that removes the 'problematic' grains identified earlier. This needs to be fed a list of problematic grain numbers, which makes it less universal for future datasets but makes it more robust for different table arrangements – in fact all it needs is for Grain No. to be in columns 1.

I completed the Turner-Weiss analysis – on the 215* new grains with 247 new twins, and hence 247 sigma 1 and sigma 3 predictions. Data is good. I seem to have picked up more sigma 1 sticking out of the image than 'up' or 'down' on the image – although these should be symmetric.

I think it's a sampling bias, but not 100% sure. May also be that deformation was not perfectly axi-symmetric, or could be a pre-existing fabric in the rock.

*Seems I missed one grain on the "Problematic grains" list, that I flagged down as problematic in the excel file.

3rd May 2021

Edit by Kamil on 04/05/2021:

I plotted all the e-poles, as well as only the resolved ones to confirm that what I saw before is just a sampling bias – it probably is.

5th May 2021

Edit by Kamil on 05/05/2021:

I started the day by figuring out how to do the inverse pole figures – the method works, but I think data needs to be adjusted for Schmid factor – else it plots all over the place.

Next, I tried working out the Schmid factor. Initial working has given me 64 grains with positive Schmid factor. That is low. I plotted them, and it happens to be the ones that should not be twinned. Perhaps it is the negative Schmid factor that I am looking for. I am trying to work it out, but the task will probably extend to tomorrow.

Solved it – I am in fact looking for negative Schmid factors in the sense that it is calculated along acute angles, but my slip vector will always be obtuse. Hence doing 180° - λ solves it, but has the same effect as switching the Schmid factor signs.

6th May 2021

Edit by Kamil on 07/05/2021:

Yesterday I counted all the twin planes in each valid grain. Easy, but time consuming.

7th May 2021

Edit by Kamil on 08/05/2021

Yesterday I fixed the two problematic grains: 181 and 283. I exported grain sizes, twin counts, and pressures to a spreadsheet.

8th May 2021

Edit by Kamil on 08/05/2021

I worked out the apparent and corrected twin densities – by using the feret diameter. Then to adjust for the dip of the twin planes relative to the plane of the image, I divided the apparent densities by the cosine of the plunge the e-pole makes with the plane. I'm now ready to split it into groups and plot.

10th May 2021

Edit by Kamil on 11/05/2021

I plotted various graphs showing relationships between the Schmid Factor, Pressure, Twinning activity, and grain size. I found that even though there is now plenty more data available, the relationships are not so clear cut. The best I found is a data-bounding envelope on the activity-pressure charts. This may or may not depend on the Schmid factor for the larger grains.

11-21st May 2021

Edit by Kamil on 23/05/2021

This time has been spent producing figures and writing the thesis itself.

27th May 2021

Edit by Kamil on 27/05/2021

Poster and presentation complete. Paper notes scanned in. All files available at:

https://github.com/Kamkosiorek/Calcite-Palaeopiezometery

https://drive.google.com/drive/folders/1Bh9hmtb2ONqP3WhJnVcO5yk0Qjknu6pj?usp=sharing

Earth Materials Chapter 4

X-ray diffraction ≠ X-ray powder diffraction

↳ perfect crystal irradiated, atomic distances learned.

Atomic radius : $\frac{1}{2}$ distance between 2 identical atoms (centres, spherical)

Coordination number = number of anions

Ca^{2+} often forms octahedral to cubic coordination

↳ $\underline{VI}$ ↳ $\underline{VIII}$

Isodemic - All bonds are the same strength

Calcite → Anisodemic ? Δ -triangles

↳ $CaCO_3$ ↳ $(CO_3)^{2-}$ polygons more strongly bonded to each other than other ions

$\boxed{\text{Figure 4.9}}$

Calcite structure: Combination of Octahedral CaO_6 ← 1/3 per O ~~2 charge~~?

and Triangular $(CO_3)^{2-}$ ← -2/3 per O

Each oxygen coordinated to Calcium AND Carbon

Some mention of ionic substitution, but I think it is not relevant.

30 OCT 2020

1 1 1 .

-1 1 1 . -1 -1 1 .

1 -1 1 . 1 -1 -1 .

1 1 -1 . -1 1 -1 .

-1 -1 -1 .

$\{001\} \rightarrow (001), (00\bar{1})$

But still two for hexagonal?

Earth Materials Chapter 5

Hermann - Maguin

Calcite: Trigonal, $\bar{3}m$, H-M : $\boxed{\bar{3}\ 2/m}$ Space group: $R\bar{3}c$

4 types of symmetry in - Mirror plane
R - Rotation axis → n = number of repeats
i - Centre of symmetry → Inversion
$\bar{R}$ - Rotoinversion axis → ~~rotat~~ rotation with inversion
← complicated

Point group elements → symmetry elements intersect in the centre of the crystal.

32 possible crystal classes

$\bar{3}$ equivalent to 3-fold rotation in combination with centre of symmetry (i - inversion)

rotational axis perpendicular to mirror

$1R_3$, $3R_2$, $3m$

$\bar{3}\ 2/m$ is Hexagonal

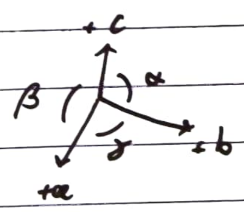
$1\bar{R}_3 = 1R_3 + i$

? Rotate 3 times → like turbine, and invert looking down?

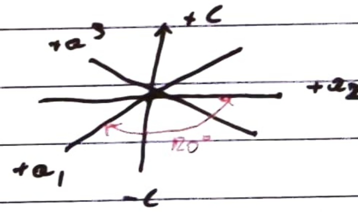
In 5 of 6 ~~cr~~ systems, 3 axes are used to describe crystal
In 1 of 6, Hexagonal, 4 axes are used:

a_1, a_2, a_3, c

hkl for undefined intercept to crystal direction



← 3 axis system



$a_1 = a_2 = a_3$ at 120°

c perpendicular to plane

(hkil) for hexagonal

Return to p95 box

Miller indecies → inverse of Weiss system. ← crosses negative axis

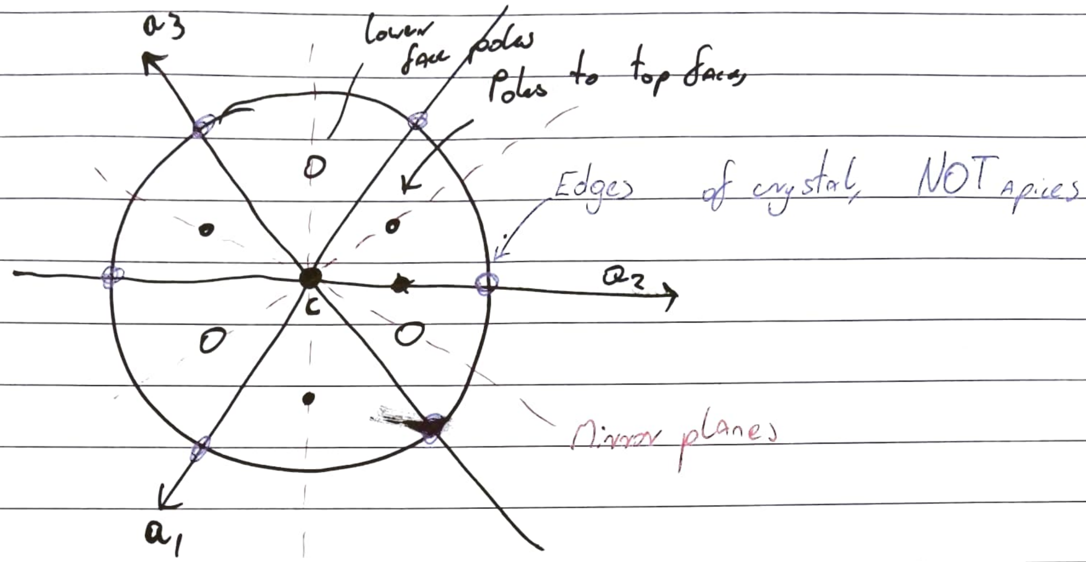
Just coordinates of surface $(\infty, \infty, \bar{1}) \rightarrow (0, 0, \bar{1})$
a b c → a b c

Different for Hexagonal system

30 OCT 2020

$\bar{3}\,2/m \rightarrow$ rhombohedron.

Parallel faces by inversion, not mirror reflection



Clinographic projections → perspective drawings of crystals,
Much better than photograph
- c-axis vertical, b axis East – west, a axis towards observer

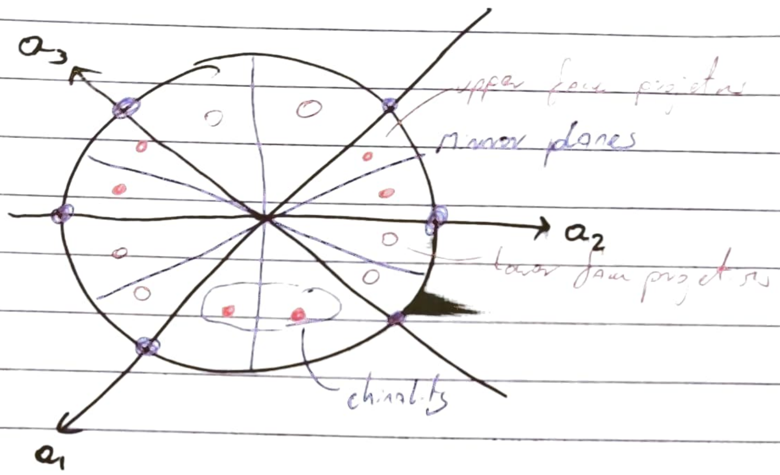
In $\bar{3}\,2/m$ ← c axis is rotoinversion, and three horizontal axes are 2-fold ~~rotat~~ rotation.

General form $\{hk\bar{i}l\}$ is a scalenohedron
↳ Closed form of 12 scalene triangles

Distinguished from ~~tet~~ dipyramid by zig-zagging middle edges

Common form, rhombohedron → $\{h0\bar{h}l\}$ and $\{0h\bar{h}l\}$
Closed form of 6 rhomb shaped faces
- Like a squished or extended cube.
~~Com~~ Rhombohedron common index = $\{10\bar{1}1\}$

In general form: (Hexagonal Scalenohedron → 6-edge di-pyramid with zig-zag edges



XRC – X-ray crystallography

Calcite wiki page

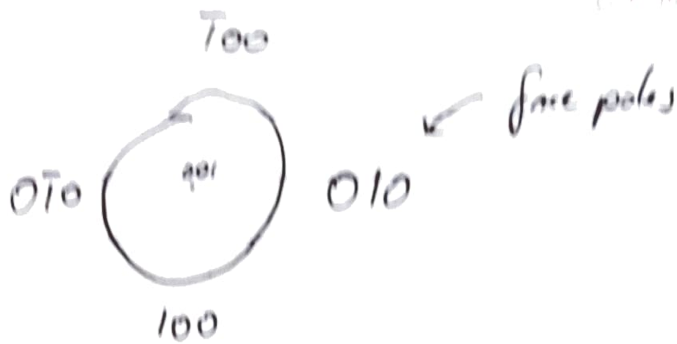
Different forms of twinning ~~depending on~~ → fibrous, granular, lamellar or 'compact'

Cleavage in 3 directions parallel to rhombohedral form

Scalenohedral faces are chiral (mirror image symmetry).
Rhombohedral faces are achiral.

In crystallography

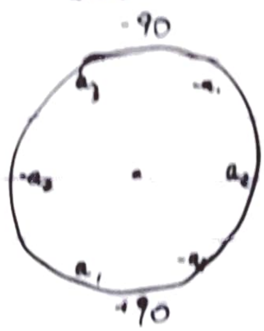
Project from upper hemisphere onto primitive circle.



But once again for 3 axis system

Wulff nets more commonly used. in crystallography

Idea from the web:



- Solid bold line = m axis
- c axis is perpendicular to page

No horizontal (primitive circle) for $\bar{3}2/m$

= c axis

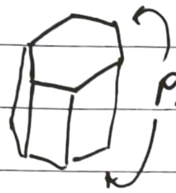
Vertical axis → ~~one~~ 3-fold rotoinversion axes. no perpendicular mirror

Mirror axis vertical and interleaved with horizontal axis?

Figure 5.9A + 5.9B

30 OCT 2...

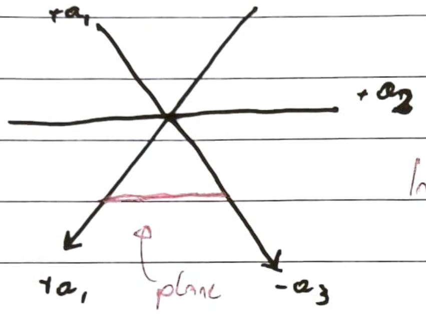
In Hexagonal system → Use Miller-Bravais index ~~notation~~



Pinacoid · Hexagonal prism

surfaces on top and bottom

Plan view



Intercepts at $(1 \quad \infty \quad -1 \quad \infty)$
$a_1 \quad a_2 \quad a_3 \quad c$

Simple enough

$\hookrightarrow (1, 0, \bar{1}, 0)$

Also $\{hk\bar{i}l\}$ for general form ← but still not sure HOW that works.

Wiki: Note: Calcite is: Ditrigonal scalenohedral. Centrosymmetric
Space group number: 162-167

What is form index?

[001] ← direction $\quad$ (001) faces $\quad$ {001} form

perpendicular to

can mean any combination of positives and negatives?

Creation of stereographic projection of a crystal first involves spherical projection of perpendiculars to each of the crystal faces (face poles)

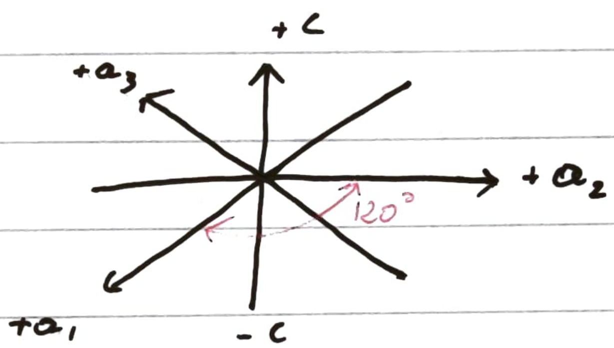
$\{001\} \rightarrow (001), (00\bar{1})$

$\bar{3}m$ is abbreviation of $\bar{3}2/m$

30 OCT 2020

Notes on calcite & crystal structures in general from yesterday:

Calcite is in hexagonal crystal structure
- Has 4 crystal axes - c, and a_1, a_2, a_3



a_1, a_2, a_3 are co-planar, c axis is normal

Calcite is anisodemic (?) - not all bonds are the same strength. Each oxygen is co-ordinated to Calcium AND Carbon

2-fold rotational axis perpendicular to mirror axis

Hermann-Mauguin notation: $\bar{3}$ 2/m

↳ H-M

↳ 3-roto inversion axis

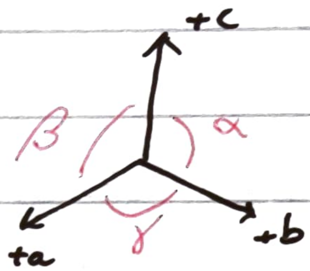
Space group: R$\bar{3}$c

So - Rotate around 3 times and invert looking down?

(Earth Materials, Chapter 4 & 5)

30 OCT 2020

For system with 3 axes (NOT Calcite):



indicates negative axis

Weiss Miller

And miller indecies are: $(\infty, \infty, \bar{1}) \rightarrow (0, 0, \bar{1})$
A b c A b c

Symmetry Key: R – Rotation axis
m – Mirror axis
i – centre of symmetry, inversion
$\bar{R}$ – Rotoinversion – rotation with inversion

Calcite is also $\bar{3}m$ – I think simpler, but less complete description than H-M

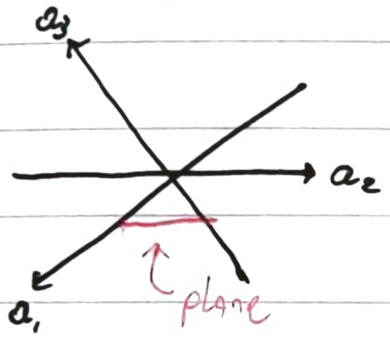
(Earth Materials, Chapter 4 & 5)

31 OCT 2020

Notes on calcite and stereonet projections

In crystallography, upper Hemisphere, Wulff net projections common.

In hexagonal systems, use Miller-Bravais index:



$\quad\quad a_1 \quad a_2 \quad a_3 \quad c$

Intercepts at $(1, \infty, -1, \infty)$

$(1, 0, \bar{1}, 0)$

in Miller-Bravais format

(001) is a face

[001] is a direction normal to that face - "face poles"

{001} is a 'form'. Means possible +/- combinations: (001), (00$\bar{1}$)

In a basic stereographic projection, face poles are projected.

$\bar{3}m$ is just abbreviation of H-M's $\bar{3}\,2/m$

Clinographic projections - perspective drawing of a crystal.

c-axis vertical, b-axis East-West, a-axis towards observer.

(Earth materials, Chapter 4 & 5)

31 OCT 2020

Few notes on calcite crystal structure/shape

- Few shapes can satisfy the $\bar{3}\,2/m$ symmetry.
- Common ones are rhombohedron and hexagonal scalenohedron, (or combination of the two) (6-face/edge dipyramid with zig-zaggy middle edges)
- Cleavage in 3 directions parallel to rhombohedral form.
- Scalenohedral faces are chiral (mirror image symmetry)
- Rhombohedral faces are achiral
- Different forms of twinning common in calcite:
  Fibrous, granular, lamellar, compact
  (Wikipedia page on 'Calcite')

Both rhombohedron and scalenohedron are closed form - faces enclose space completely

General form $\{hk\bar{i}l\}$ is a scalenohedron, 12 scalene triangles

Common forms for rhombohedron: $\{h0\bar{h}l\}$ and $\{0h\bar{h}l\}$
- 6 rhomb faces, like squished or elongated cube
Common rhombohedron index is $\{10\bar{1}1\}$.

(Earth Materials, Chapter 4 + 5)

31 OCT 2020

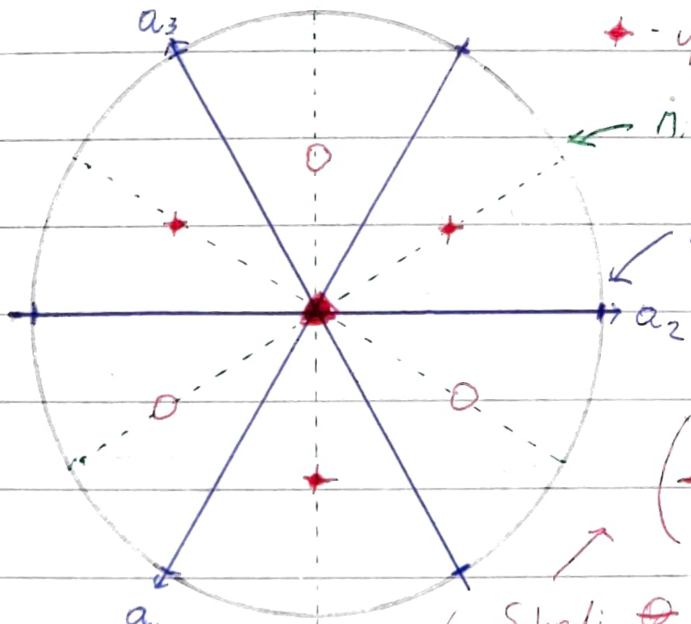
Stereonet projections:

In $\bar{3}$ 2/m, c-AXIS is the rotoinversion axis.
Horizontal axes are 2-fold rotation

In the rhombohedron form, (and maybe scalenohedron too), parallel faces are by inversion, NOT reflection

Rhombohedron:

o - lower face poles
✦ - upper face poles



Mirror planes

Edges of crystal, not Apices.

▲ is the c-AXIS

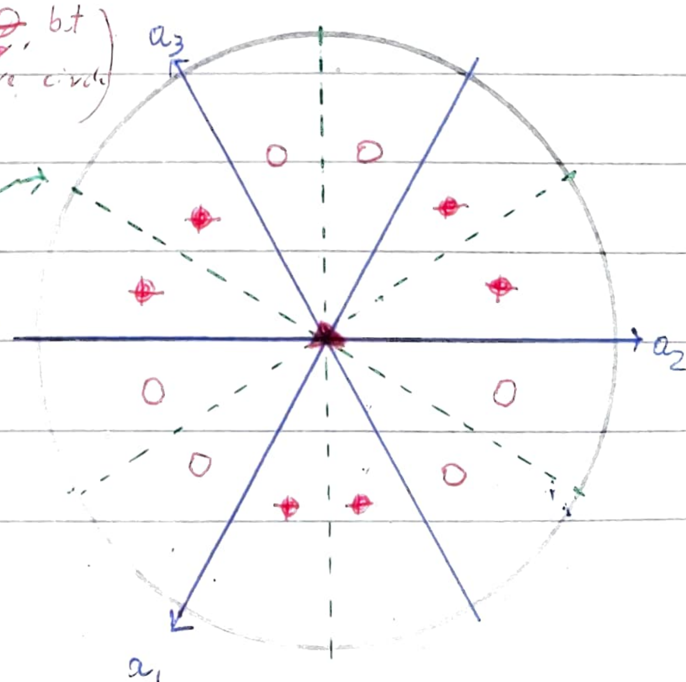
(If upper hemisphere projection used, why not $a_1 \leftrightarrow a_3$???)

(Solved: ⊖ but look at primitive circle from above.)

Hexagonal Scalenohedron:

Mirror planes

pretty sure ~~also~~ the EDGES, not apices.



o - lower face projections
✦ - upper face projections

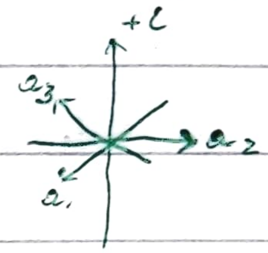
(Earth Materials, Chapter 6)

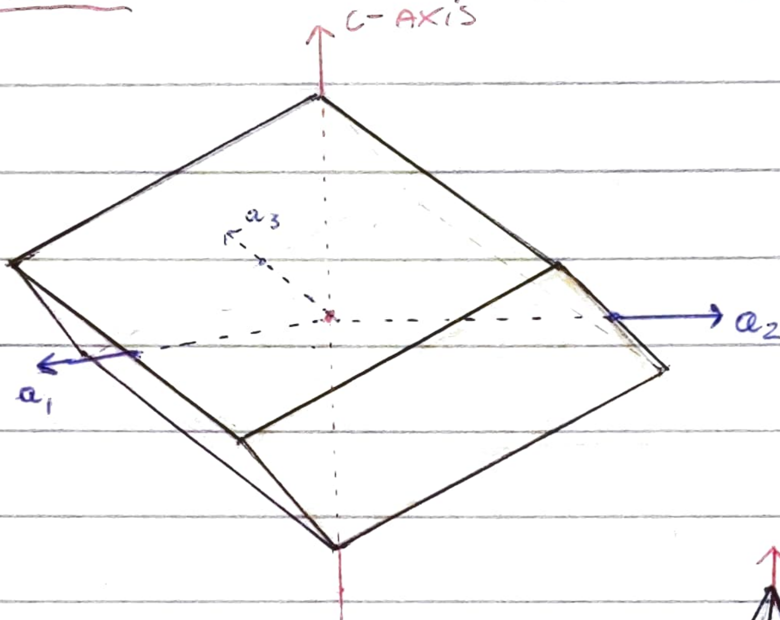
31 OCT 2020

Two common forms of Calcite drawings

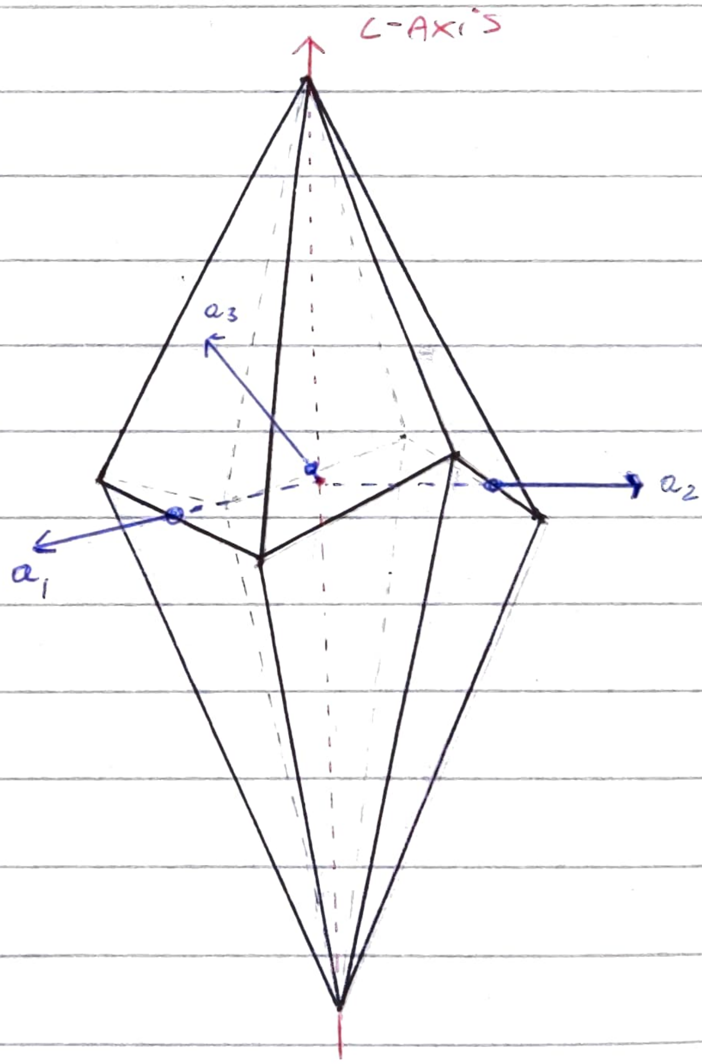
Rhombohedron:

(clinographic projections)





Hexagonal scalenohedron:



- Both have C-AXIS exiting through an apex
- Both have Horizontal axes exiting through edges

(Earth Materials Chapter 6)

↗ NOT already present

07 NOV 2020

Twin element → New shared symmetry element
- Mirror plane or twin plane
- Rotation axis or twin axis
- Inversion about a point or twin centre

} Twin laws

For Growth twins ← Deformation is not a growth twin?

Interested in Secondary twinning

Classification of twins:

Contact ~~tw~~ twin → separated by twin plane

Penetration twins → Appear Intergrown → Axis of rotation common

Multiple → 3 or more crystals twinned, according to laws

Polysynthetic twin - All composition surfaces are parallel

Ref of chapter 5 if needed ⇒ Bravais notation

Re-watched on: 04 MAR 2021

(1)

1st Lecture with Ernie:

Dynamic recrystallization: Calcite recrystallize at high stresses
Bigger stress → smaller grains

c-Axis → trigonal rotation axis
Trigonal system → hollosymmetric class

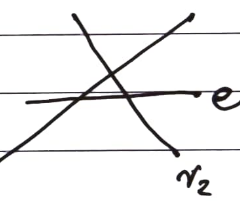
No centre of symmetry → piezoelectric properties (Qtz)

Calcite has centre of symmetry → no piezoelectric properties

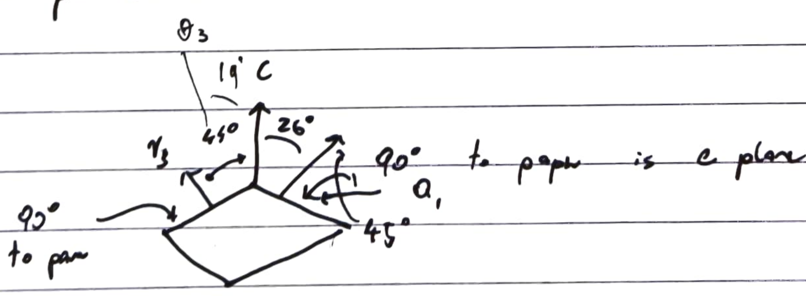
Nomenclature for calcite (rhombohedral)

→ faces called (r_1, r_2, r_3)
→ steep faces (spar-type) (f_1, f_2, f_3)
→ basal (c)

e plane → halfway between r_1 and r_2
parallel to ~~apex~~ edge
twinning plane



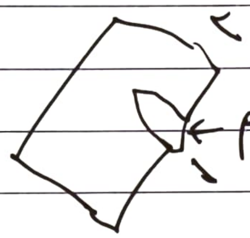
Each parallel to Edge between r planes
3 e planes



Positive sense of twinning → moves upper towards c-Axis.
THE Only possible sense of twinning

② 04 MAR 2021

Shearing can produce twinning - Martensitic transformation



propagation twin lamellae

In calcite only 3 slip systems (e_1, e_2, e_3)
Need 5 to satisfy Taylor - "phenomenon" → need N planes
'~~von Mises~~' ?

Smaller crystal harder to twin as backstress (from surface energy) fights against it.

Small enough grains don't twin

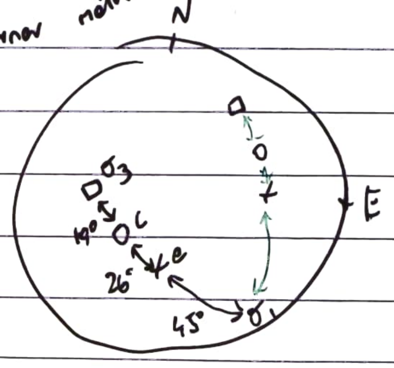
- Shearing in opposite sense is not possible.
Will de-twin already twinned calcite.

Optimum direction of compression at 45°

If see a twin → assume optimally oriented

Plotted on stereonet will give directions of σ_1 & σ_2

Turner method



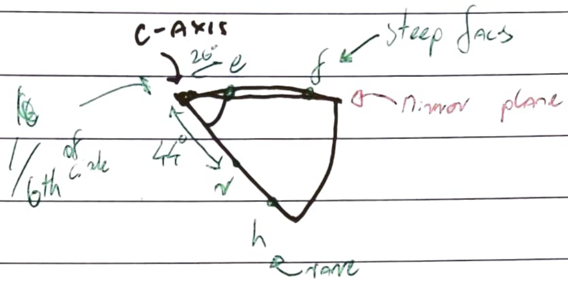
Multiple sets of grains can tell σ_1

- Think about good reference from pole figure

③ 04 MAR 2021

On Ernie's paper:
(Ritter, 1994)
+ Casey + Burden

Or relate geographic axes to crystal axis → "Inverse pole figure"



To link crystalographic axes to outside world
- 9 direction cosines, 6 of which independent
- 3 Euler angles (0 - 180°)

σ_1 s should cluster around a point

From cluster → harmonic (spherical function fit
"Orientation distribution function"

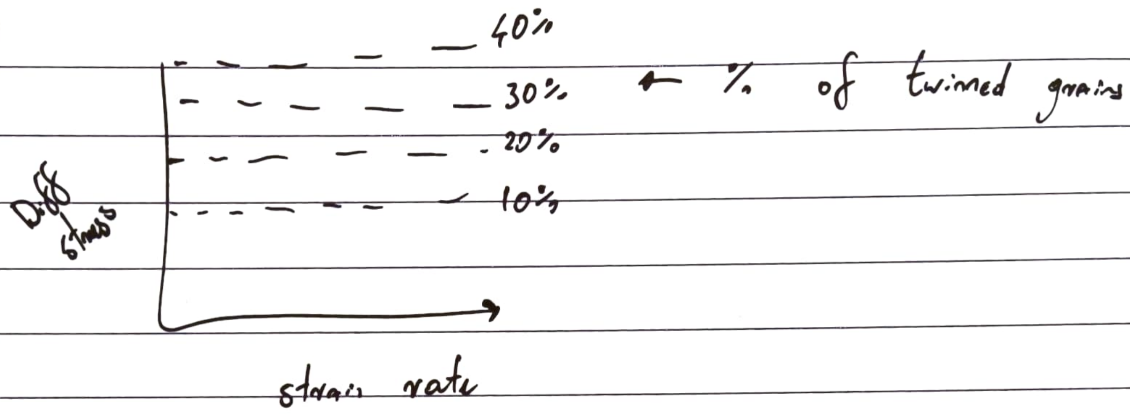
Inverse-pole figure is a section of ODF.
→ back-calculate data to check GoF

At higher temperature natural weaker →

E-maximum fabric → low temp, twinning dominated
E + Ah fabric → not to do with twinning ← Sudden flip at certain conditions

Twinning forms in compression

4



• FIND PLANAR GRAIN SIZE DISTRIBUTION

2 Problems with palaeo piezometry :
- Determination of orientation of $\sigma_1, \sigma_2, \sigma_3$
- Determination of magnitudes.

• Twin boundary migration can have some effect.

→ In EBSD → Test for twin :
72 degrees between crystallography and a twin ?
↳ ~~[illegible]~~

Twins + slips on r+f may cause rotations in host grain
< 10° variation for Heterogeneous strain

Aim: Extract a good parameter describing twin activity
eg. - Twin density
- Twin number
- Thickness (etc)

Schmid factor:
- Does not work well for twinning because of grain size effects on twinning stress

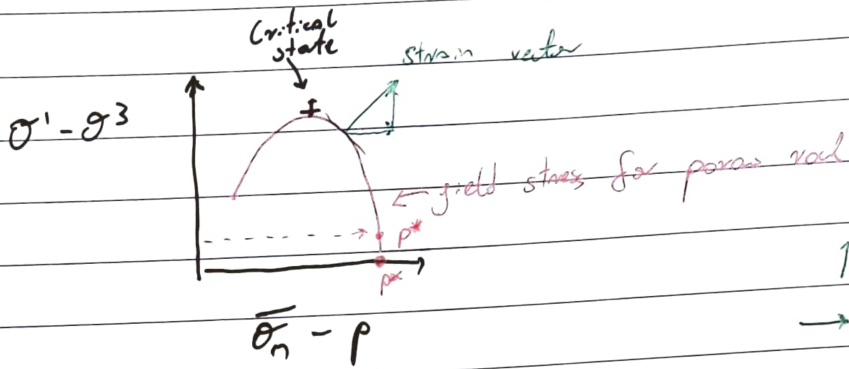
Aim
Extract good Palaeopiezometer

0 4 MAR 2021

(5)

Yield stresses → Crystal-plastic → → 2 models

Strain vector normal to criterion



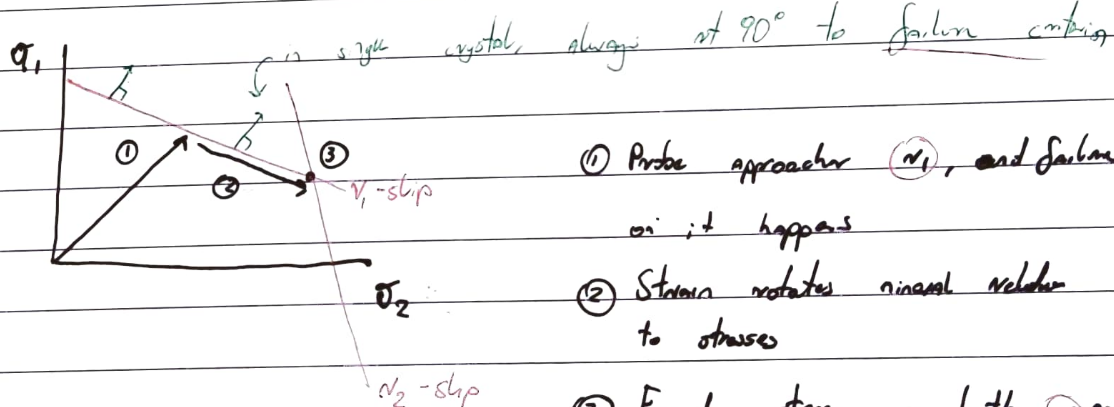
↑ Distortion strain

→ Volumetric strain

But often strain vector not ⊥ to failure criterion

"Non-associated flow"

For single crystal:



(1) Probe approaches ν_1, and failure as it happens

(2) Strain rotates normal relative to stresses

(3) Equal stress on both ν_1 and ν_2 slip systems

(4) In 3D, travels long edge to a vertex

(5) And so on into 5-dimensional space

(Taylor, Bishop, Hill analysis)

Carrara Marble → Relatively free of Twins to begin with

1978 paper ← 5 dimensional stress

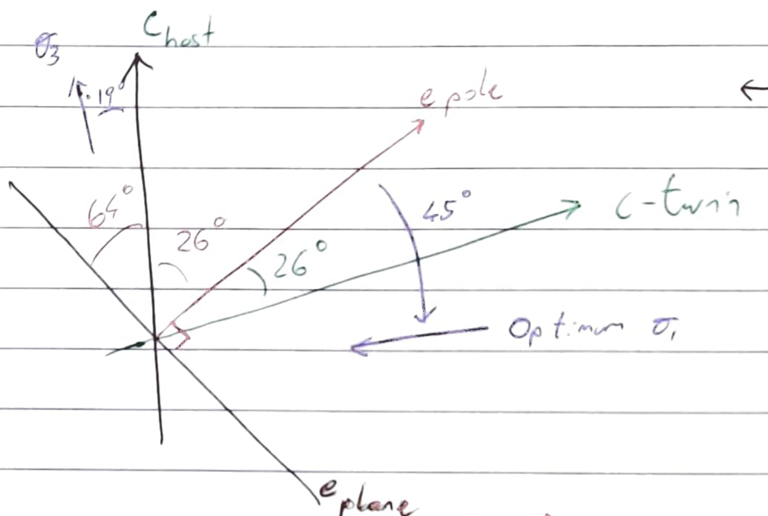
↳ Blister William textbook too

PLAY WITH DATA!

① 05 MAR 2021

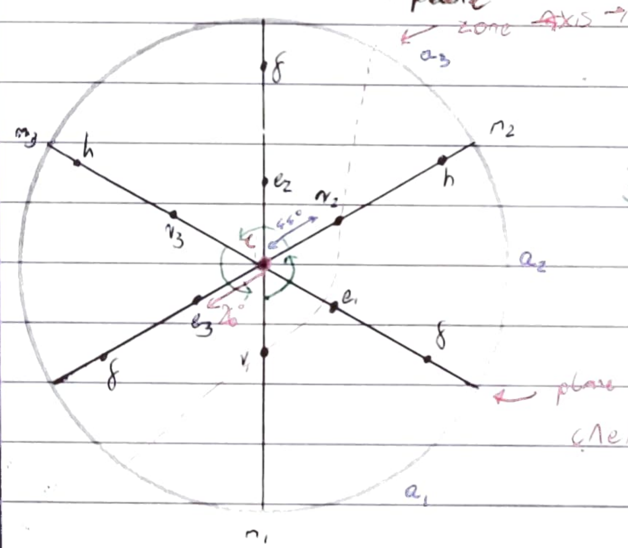
Second Meeting with Ernie.

Try MTEX for all plotting



← View onto cnenf zone

c of twin reflected about E



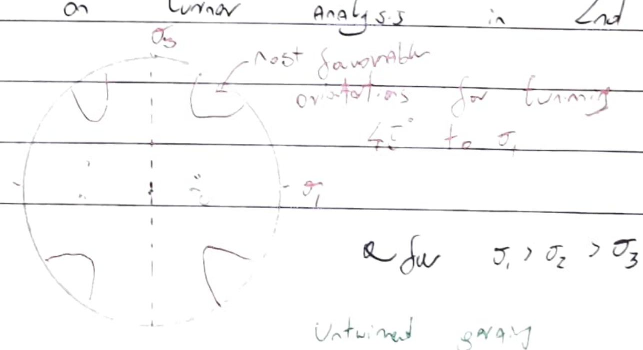
3 segments repeated by rotation
Bisected by mirror symmetry

← plane called cnenf zone (also called axis)

Slip deformation important for fabric / deformation at high temp.
At low temp → stay in twinning mode

Use Wulff (equal Angle net)

More on twin analysis in 2nd lecture



05 MAR 2021

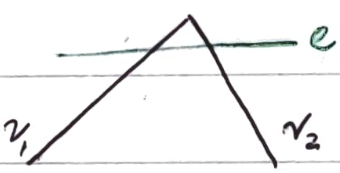
Few more notes about Calcite

(based on both meetings with Ernie)

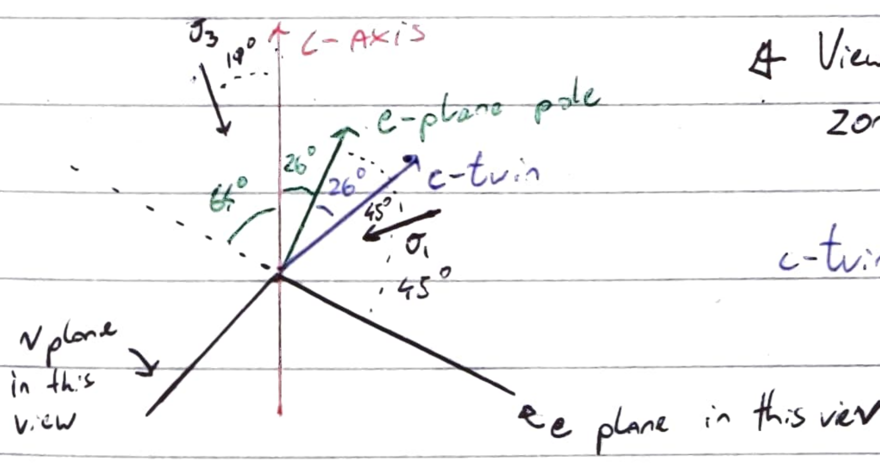
Faces and other planes have particular nomenclature:

- faces are called "r_1, r_2, r_3"
- steep faces are "f_1, f_2, f_3"
- basal faces are "c"

"e" plane is a twinning plane, which lies halfway between two "r" planes:



e-plane is parallel to non-a edges in rhombohedron.



⇐ View onto the c∧e∧f zone

c-twin effectively reflected around e-plane.

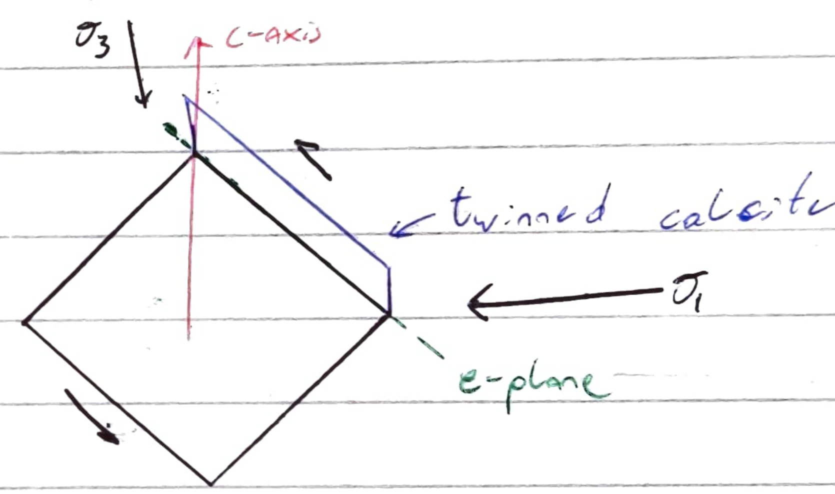
both ⊥ to page

σ_1 is at 45° to e plane.

05 MAR 2021

Notes on calcite continued:

- Calcite twinning allows for only 3 slip-systems. That is, there are only 3 e-planes.
- Need 5 to satisfy 'von Mises' criterion (if no volume change).
- Hence some slip must occur on r or f or other planes.



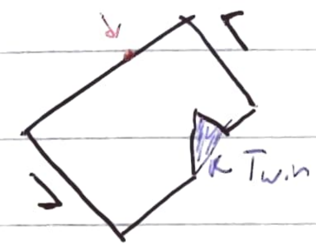
- Only positive sense of shear is possible in Calcite (Towards the c-Axis).

- In the other sense of shear, calcite will not twin, and even de-twin if already twinned

Hence, if see a twin, assume it is optimally oriented!

0 5 MAR 2021

Twinning in Calcite



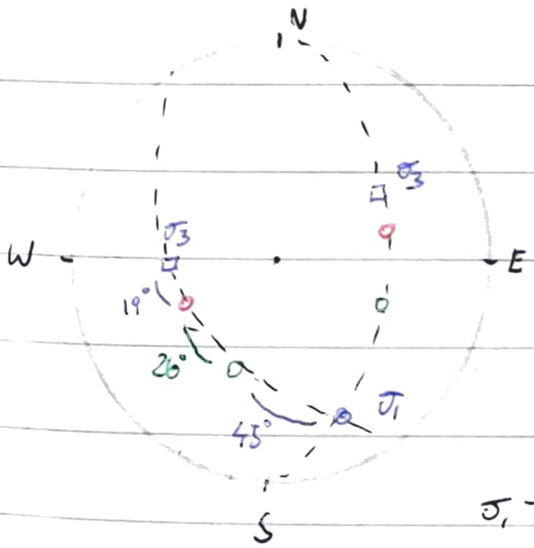
- Twins propagate through the crystal as "wedges", but are opposed by the "backstress" caused by the surface energy at the other side of the crystal.

Hence, bigger crystals Twin much easier than smaller crystals.

At high strain rates, calcite undergoes "dynamic recrystalisation" which reduces the grain size and potentially removes twins.

Turner Method - Strongly simplified

Turner method tells us the σ_1 and σ_3 directions.



① Plot c-Axis for few host grains

② Plot e-poles for those grains

③ Plot σ_1 45° from e and σ_3 19° away from c.

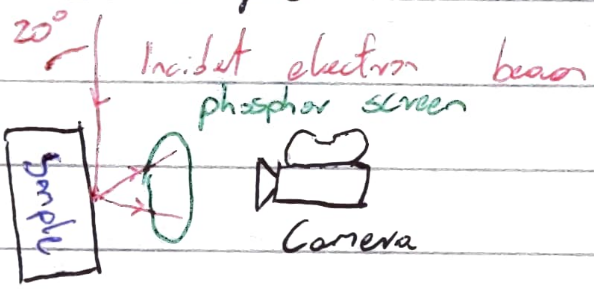
σ_1 - should cluster in one area.

σ_3 may be spread if stress Axi-symmetric

08 MAR 2021

Notes on EBSD

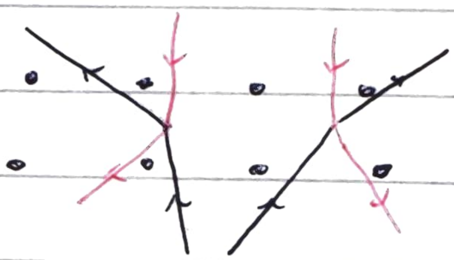
- Electron back-scatter diffraction gives us the orientation of a crystal within a sample

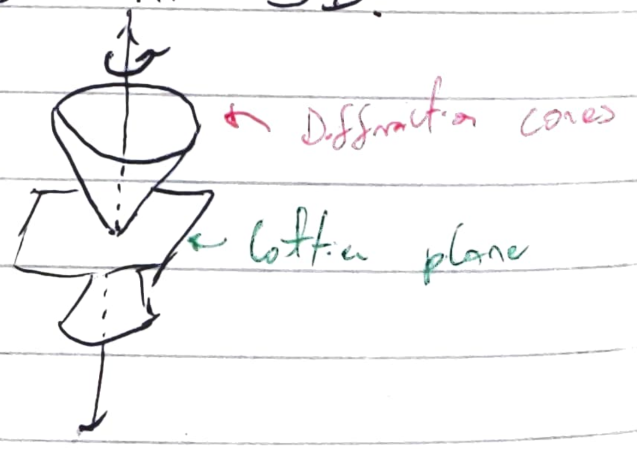


1. Electron beam hits the sample at a shallow angle

2. Interaction within upper μm's of the sample create an omnidirectional source of electrons

3. Electrons are diffracted by the near-surface lattice planes. There are 4 possible paths satisfying the Bragg equation in 2D, which translate to two cones in 3D.





* Meant to be symmetrical

08 MAR 2021

Notes on EBSD continued

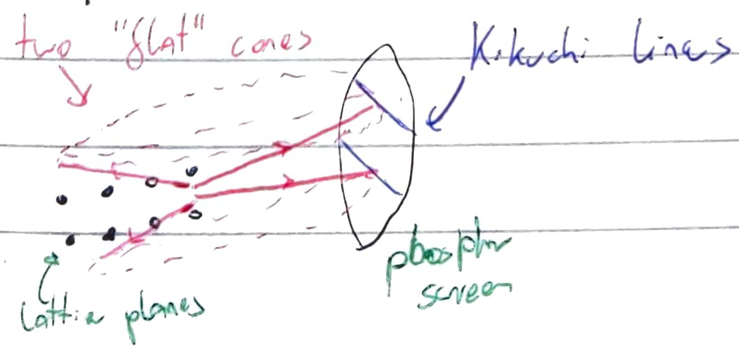
4. At the electron energies typically used in EBSD, the diffraction angles satisfying the Bragg equation,

$$n\lambda = 2d \sin\theta,$$

where n is the order of diffraction,
λ is the electron wavelength
d is the lattice spacing
and θ is the Bragg angle

~~the~~ ~~the~~ are typically pretty shallow. In fact, they are almost 90° and the two cones are open at about 180°

5. The two almost-parallel planes hit a phosphor screen and produce a Kikuchi patern



08 MAR 2021

Notes on EBSD continued

6. The image produced on the phosphor screen is captured by a CCD camera.

7. The bisectors of individual Kikuchi bands are the projections of lattice planes.

8. Computer uses Hough transforms to process the data and index (compare) the pattern to a known database.

9. Once orientation is known, Process is repeated at the next site, eventually producing a map of crystal orientations.

The process usually takes place within an adapted Scanning Electron Microscope (SEM)

12 MAR 2021

Ernie's 1989 paper notes

Found link between : Diff stress and twinning incidence
Density + Volume fraction
Grain size control

Verify Ernie's data in my findings

Turner 1953 for Turner method
(Turner Dynamic Analysis) - TDA

Good review by Turner & Weiss 1963

Testing apparatus might be ~~outlined by~~ described by Rutter 1972 or 1985

Low (<0.2%) porosity

Carrara relatively untwinned

Induced twins tend to be Lenticular

Readings based on 200-300 grains

Twinning Largely independent of strain rate and Temp but Sensitive to stress

Not thermally activated. Ideal for Paleo stress indicator

~20% of grains expected to not show twinning - unfavourable orientation

Twin density is independent of Grain size
& dependent on stress

12 MAR 2021

Schmid factor, m

$$m = \cos\phi \cos\psi$$

Normal between ~~maxim compression~~ ~~maxin~~

$\phi \rightarrow$ Angle between maximum compression direction and normal to twin plane

$\psi \rightarrow$ Angle between compression direction and twinning displacement vector

Resolved shear stress maximised when both at 45°

$0 < m < 0.5$

Volume of twin analogue is indepent of deformation history

Found it is good analogue to natural rocks

Volume, hardness, and Density all useful

for simpler history, more accurate

13 MAR 2021

Ernie's Q3 paper

Crystalographic Orientation development during deformation

Strain deformation is good because stress is always homogenous

In compression, stress not necessarily ~~pr~~ proportional to cross-sectional area

At 300-500°C flow is strain-hardening

A low temp, ~~[illegible]~~ flow insensitive to grain size
<600°C

At mid temp, mid stress, flow becomes grain size sensitive
600-700°C

Twinning easier at larger grain size

→ Natural rocks almost always show e-fabric?
(Low temp)

Impurities strongly inhibit calcite recrystallisation

Twinned Calcite rock ~~[illegible]~~ anneal back to equigranular at high temperatures → Twinning gone but CPO present

CPO fabrics can survive subsequent deformation

13 MAR 2021

Intracrystalline Plasticity (A) is what interests me
(e-fabric)

04 Rutter

15 MAR 2021

Distribution of non-plane strain - Solnhofen

- Short cylinders (radius > length) length half the radius
  ↳ Non-plane strain → heterogeneities present

Crystal plasticity as deformation mechanism

SPO ← Shape preffered orientation

← middle parts extruded

Vorticity occurs (in flow)

Shape fabric

Specimen diameter → 9.5mm

Good diagram of pizza slice with Miller-Bravais indices on it

In general, shows CPO from EBSD data transect across a sample deformed in multiple regimes

Still no et al in natural rocks

15 MAR 2021

Very crude notes on Evnics '89 paper

→ There is a link between Differential Pressure and:
- Twinning incidence
- Twining density
- Twin Volume fraction

(Also found that there is a grain size control - small grains don't twin)

(I should confirm the same relationships in my data)

→ Twinning largely independent of strain rate and temperature, meaning twinning is not thermally activated ← great palaeopiezometer

→ Only favourably oriented grains twin. About 20% of grains expected to not show twining as they are unfavorably oriented.

→ Induced twins tend to be more lenticular

→ Twin density is independent of grain size, but still dependent on stress

→ Twin volume fraction analysis is independent of deformational history

15 MAR 2021

Crude notes on Ernic's '93 paper

- Lists advantages of deformation in extension, but those do not apply to my study.

- Twinning is easier at larger grain sizes.

- At 300-500°C, flow is strain-hardening. Low temperature is important, as that's where the e-fabric develops

- Natural rocks show e-fabric only

- Twinned calcite rocks anneal back to equigranular structure at high temperatures. Twinning disappears, but CPO remains

- Those CPO fabrics can survive subsequent deformations

- Intracrystalline plasticity is the term from this paper that interests me. It leads to e-fabric

16 MAR 2021

Rutter 14

- Because most minerals are seismically anisotropic, a rock with a CPO should too show an a seismic anisotropy

- Mention 5 slip systems

- Crystal lattice ~~on~~ rotates (along with slip system) as slip occurs until at "easy slip" + steady orientation, easiest slip

- Conjugate shear systems can cause assymetry
- Can somehow use this assymetry in flow analysis?
- 3D analysis at various points in rock should give good image of stresses in rock + whatever the deformation regime each part experienced

Once again, impurities prevent recrystallisation → Allows deformation at higher temperatures than otherwise possible

↳ Hence possibility of more slip systems + grain boundary sliding

→ Interesting seismic properties of calcite

→ Showed CPO has an effect on seismic anisotropy

Extension → High confining pressure and withdraw pistons

→ Conditions such that Solnhofen deforms in Intracrystalline plasticity regime

Twinning in some larger grains

16 MAR 2021

Seismic properties calculated, not observed?

In calcite, V_p lowest parallel to c-axis

- Use intensity of poles to f-planes to measure the strength of CPO + but for extension?

→ Talks about how to estimate strain in compression

→ Intensity does not increase systematically with shortening

Kern 1977 1979 + Showed CPO in Limestones

- Neither patterns or their intensities correspond to nature
  e In nature, crystallisation operates

Links to Rutter 1976, 1990, 2007

NOT ABOUT TWINNING IN THIS PAPER

Don't think this paper relates much to what I am doing except maybe the f-plane IPF ~strength CPO C.A

In nature, Calcite provides more slip systems than other rock-forming minerals

↗ NW India

18 MAR 2021

Rutter → Karakoram 2007

- Karakoram fault ~~Shear~~ has a mylonite which shows ductile deformation (intracrystalline plasticity)

- Only 40-150 km

- Of interest here → Pangong range cutting through Karakoram terrane → Deep ~~A~~ crustal rocks

3mm/year on strike/slip

Quaternary slip rate on ~~B~~ Pangong estimated at 4mm/year

Low seismicity and long recurrence rates

- 15Ma leucogranites sheared ~~→~~ faulting younger than that

Paper tries to Establish P-T history

Calcite (Marble) exposed at Muglib

USED TURNER Analysis to Produce beach ball diagrams
- Can I do this for my analysis?
Exactly what Ernie did

Twins only in coarse grains

Twins
Can tell pressure, provided the event did not cause recrystallisation
Ask Ernie

→ CPO develops c-axis ⊥ to foliation
→ Common fabric for shears and uniaxial shortening

18 MAR 2021

→ Sample 6km from fault trace has all-grains twinned

No dynamic recrystalisation found

→ Cataclastic fragmentation observed any CPO

Conclusions: Transpressive ← No surprises → //\\//

Grain-size sensitive flow by Walker 1990 ← Might be important

Archizone — Epizone??? ?
Diagenesis → Metamorphism ← Metamorphic zone

Steve and Ernie worked on Naxos, Greece marble 1989

Good: → Twinning good despite +/- 30 Mpa errors, as strain rate and temp independent

BUT GRAIN SIZE IMPORTANT

→ Fig 8

Links slip zone width to slip rate

Wider zone = higher slip rate

19 MAR 2021

Brief Notes on Ernie's '07 Karakoram paper

- Example of a practical application of Calcite palaeopiezometry
- Used Turner analysis on marbles in a wide shear zone to produce several "beach-ball" diagrams mapping the shear zone
  ↳ perhaps I can try to do this for my analysis?
- Method only works if rocks did not dynamically recrystalise — Ernie thinks this is an example of such rocks
- Found that Calcite is a good palaeostress indicator despite 30MPa error bars, as it is strain rate and temperature independant.
- But as always, it is grain-size sensitive and that must be taken into acount.
  ↳ Probably need to produce grain-size distributions for my analysis.

19 MAR 2021

Brief notes on Ernie's '14 paper

- Looks at seismic anisotropy in Calcite crystals, and calcite rocks with a CPO

- c-axis is the slowest seismic direction in Calcite

- Perhaps a useful link between poles to δ-planes and IPF to provide a measure of CPO strength
  ↳ Not sure if applies to my "type" of deformation though

- In general, I don't think this paper relates much to what I am doing.

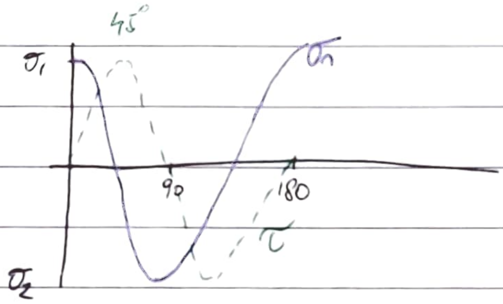
①

26 MAR 2021

Geomechanics for petroleum engineers

Heterogenous stress → Stress trajectory orientations vary from place to place
If they converge component increases in value

Shear stress numerically at maximum at 45° to principal stress



$\sigma_n = \frac{1}{2}(\sigma_1 + \sigma_2) + \frac{1}{2}(\sigma_1 - \sigma_2)\cos(2\theta)$
$\tau = \frac{1}{2}(\sigma_1 - \sigma_2)\sin(2\theta)$
↑ θ is the normal of a plane measured to $\sigma_{1,2,3}$

Homogenous Strain → Straight lines remain straight, parallel lines remain parallel, but angles change

Young's modulus : $E = d\sigma_1 / de_1$ (stress, strain) Poisson ratio: $v = e_x / e_y$

Individual strains: $\varepsilon_1 = \sigma_1/E - v\sigma_2/E - v\sigma_3/E$
$\varepsilon_2 = \sigma_2 - v(\sigma_1 + \sigma_3)/E$
$\varepsilon_3 = \sigma_3 - v(\sigma_1 + \sigma_2)/E$

(2)

Wave velocities:

$$V_p = \left(\frac{K + (4\mu/3)}{\rho}\right)^{1/2} \qquad V_s = [\mu/\rho]^{1/2}$$

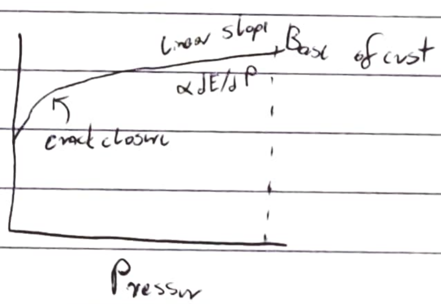
K is the bulk modulus:

~~Rigidity~~

$$K = \frac{d\sigma_m}{\underset{\text{volume}}{d\varepsilon_v}} \quad \text{or} \quad K = \frac{\overset{\text{Young's modulus}}{E}}{3(1-2\underset{\text{poisson's}}{\nu})}$$

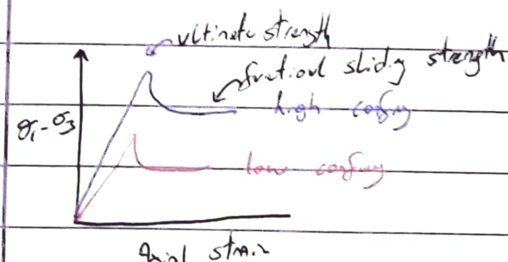
μ is the shear modulus (G)

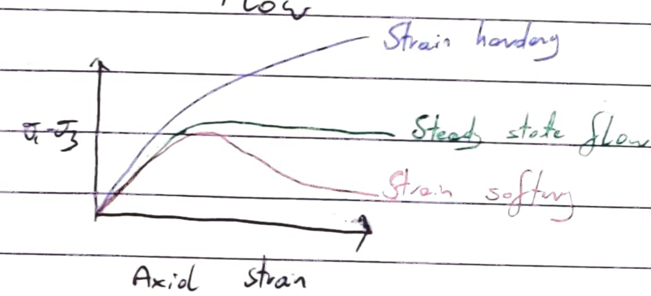
$$\mu = G = \frac{d\tau_{ij}}{d\gamma_{ij}} = \frac{\overset{\text{Young's modulus}}{E}}{2(1+\underset{\text{poisson's}}{\nu})}$$



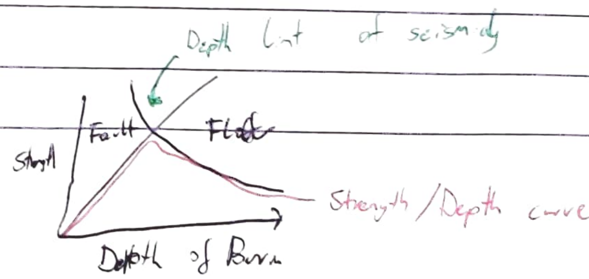
Rocks begin to flow above 300°C (salt at 80°C!)

Faulting vs Flow





In crust:



~~8~~ 3

26 MAR 2021

Creation of cracks requires volume increase. This becomes harder with depth because of increasing confining pressure. Shear stress must be high to overcome that. Pressure insensitive.

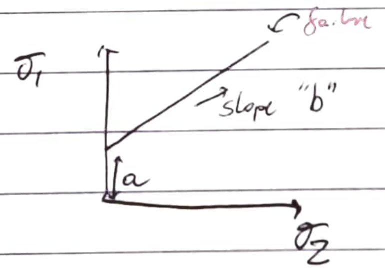
At greater depths temperatures increase and plastic flow becomes easier. Plastic flow preserves volume and so is pressure insensitive

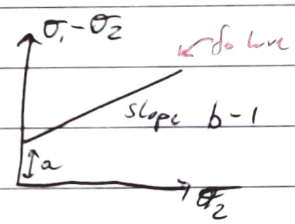
One principal stress can be expected to be perpendicular to ground surface as $\tau = 0$

faults at 30° to σ_1

σ_2 lies in fault plane

Mohr - Coulomb failure ← for low porosity rocks in upper crust





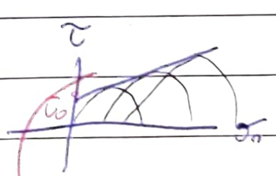
commonly 100MPa → commonly 4

Usually a straight line → $a + b\sigma_2 = \sigma_1$

Cohesion =0 for sliding on existing fault

"Unconfined Compressive Strength" for intact rocks

These plotted on Mohr circle make a "Mohr envelope"



$\tau = \tau_0 + \mu\sigma_n$

τ_0 is the cohesive strength (intercept)

μ is the coefficient of friction (gradient)

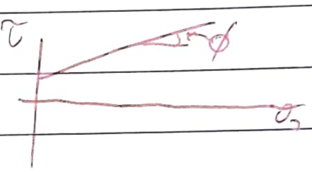
(4) For transformations:

26 MAR 2021

$a = 2\tau_0 \sqrt{b}$ $\qquad b = \frac{(1+\sin\phi)}{(1-\sin\phi)}$

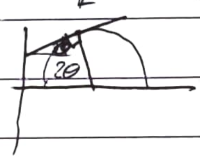
$\mu = \tan\phi$

ϕ slope of the envelope from horizontal. Usually ~30°



Angle of fault to σ_1 is $\theta = 45 - \phi/2$:

Geometry works out



Pore fluid pressure brings circle to the left

Or: $\tau = \tau_0 \mu(\sigma_n - p_f)$

pore fluid pressure

On overpressure:

$\lambda = \rho_{fluid} / \rho_{rock} = 0.4$ if pores connected to surface

μ tends to be 0.6 to 0.75

@ Byerlee's rule

Hydraulic fractures propagate in plane normal to σ_3

Mohr-Coulomb requires work to be done to create 1-2% dilation

↳ Hence rocks get stronger with depth.

↳ Works for porosities less than 10% → Otherwise more complex

(5)

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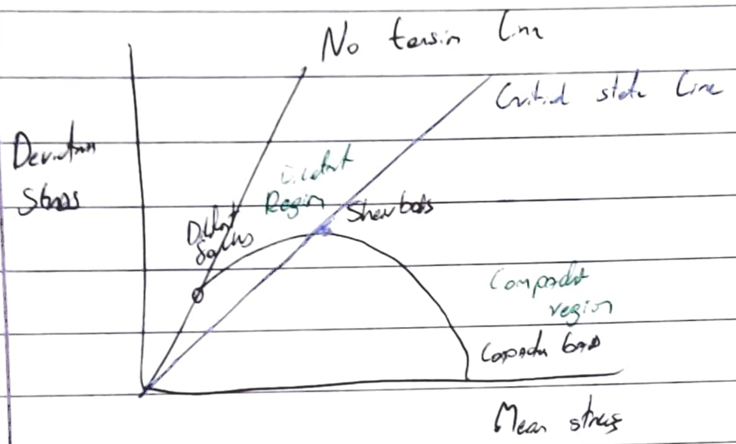
Arrhenius State Law:

$$Rate \propto e^{(-H/RT)}$$ ← Not sure what H is



Poissons ratio of ~0.5 assumes viscous fluid

Finished Near Kirsch equation

(1)

Geomechanics for Pet Eng PDF

a) Body forces → Force per unit volume

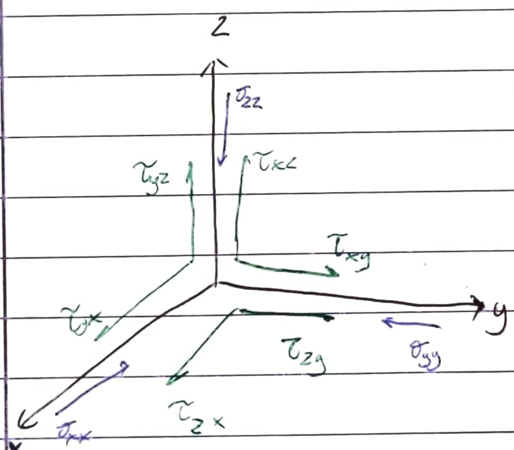
b) Surface forces → per unit area → ~~Force~~ ~~or~~ Stress or Pressure

Conventions:

Normal stress → Compression → Positive
Shear stress → Right-handed → Positive

In 3D:

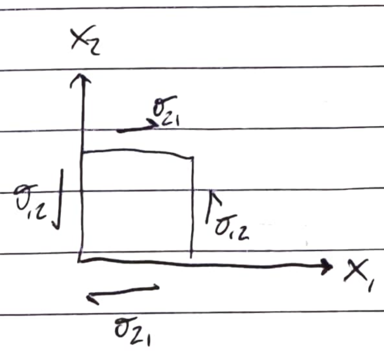
- First subscript is the Normal to the plane across which component acts
- Second subscript is the Direction in which the component acts



*Have doubts about τ

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix}$$

Stress is a tensor quantity



$\tau_{ij} = -\tau_{ij}$ ← Symmetric about leading diagonal

2

27 MAR 2021

Always possible to find orientation so that shear stresses are = 0

Orthogonal grid = "Stress trajectory"

Basically parametric equations for a circle, hence Mohr

$$\sigma_n = \frac{1}{2}(\sigma_1 + \sigma_2) \pm \frac{1}{2}(\sigma_1 - \sigma_2)\cos(2\theta)$$

$$\tau = \pm \frac{1}{2}(\sigma_1 - \sigma_2)\sin(2\theta)$$

θ is angle of plane to σ_1

τ at max when $\sin 2\theta = 1$, or $\theta = 45°$

Parametric equations to a circle

$$x = C \pm r\cos\alpha$$
$$y = \pm r\sin\alpha$$

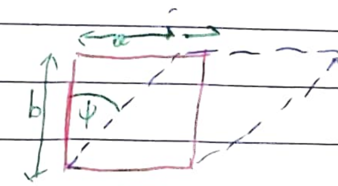
Strain:

Strain of line: $e = \frac{\Delta l}{l_0}$

Quadratic elongation: $\lambda = (l_1/l_0)^2 = (1+e)^2$

Natural or logarithmic strain $\varepsilon = \ln(1+e)$

Shear strain, $\gamma = a/b = \tan\psi$



Elasticity ~ up to 1% strain

(3) Elastic moduli

Young's Modulus $E = \partial\sigma_1 / \partial\varepsilon_i$

Shear modulus $G = \partial\tau_{ij} / \partial\gamma_{ij}$

Bulk modulus $K = \partial\sigma_m / \partial\varepsilon_V$

Poisson's ratio $\nu = \varepsilon_x / \varepsilon_y$ ← for load applied in y direction

↳ 0.5 = Isovolumetric

for rocks ~ 0.3 ← Assumes volume reduction

P waves twice as fast as S-waves

~~@ 6.5 km/s~~

$\rho \sim 2700 kg/m^3$

Typical pressure gradient: 35 MPa/km

At Moho → 1 GPa

---

04 APR 2021

<u>Intracrystalline plasticity</u>: Slippage of atomic planes one over another

Simple shear, constant volume. Pressure insensitive

↳ Surely not?

Most common deformation mechanism in lower crust

↳ At shallow depth salt does this

Dynamic recrystallisation starts around grain edges

↳ ~~Green~~ Replaces strained structure with unstrained structure

0 4 APR 2021

4

Higher stress = Smaller grain when recrystallised

Spiers 1980

04 APR 2021

What is Von Mises / Taylor Condition?

Stress homogeneous

e poles are $(01\bar{1}2)$

fabric forms as ~~slip~~ twin on e and slip on r

Host grain c-axes rotate towards σ_1

c-axes already at near $\parallel \sigma_1$ migrate to 20-30° small circle

Also no twins - kink band

Slip on r instead

Shear strain for twinning

$\gamma_t = k V_t$

Volume fraction of twin

0.694 for calcite + shear strain for complete twinning

Intensity Schmid factor for twinning groups

Twinning so easy, we don't need 5 modes as XX theorized

06 APR 2021

Euler Angles →

M → X E_3 ?
a → y E_2 ?
c → z E_1 ?

Clockwise is default → Initial anticlockwise,
Restoration clockwise

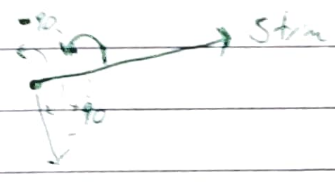
Bunge: 2 × 2

ψ_1	About	z	Axis,	-180° to	180°
θ	About	x	Axis,	0 to	180°
ψ_2	About	z	Axis		

They are rotations which bring lab in coincidence with crystal

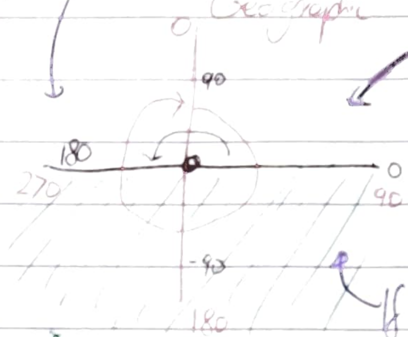
Try Again: E_1 = Azimuth strike (but may be 90° off cause diagram)

E_2 = Plunge (as on diagram) but if more than ~~180~~, 90°, flip azimuth by 180



With E_1:

If E_1 90-180, Azimuth $= 270 + (180 - E_1)$



If E_1 0-90, Azimuth $= 90 - E_1$

Actually this is my "strike"

Burge

If E_1 90-180, Azimuth $=$
0-(-90)

Never get in this zone initially.
Will do later when $E_2 > 90$

Also, if $E_2 > 90$, Azimuth gets extra +90°

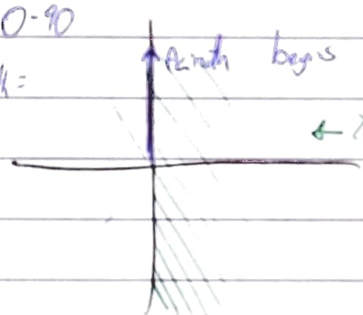
Then if >360, Do -360

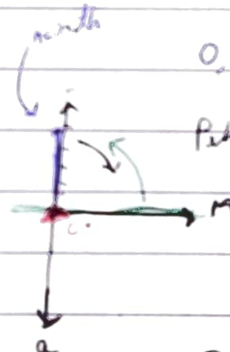
~~The~~

Plunge: If E_2 over 90, dip $= 180 - E_2$

Else dip $= E_2$

If 0-90
Azimuth =





$360 - E$

0, 90 → ~~$90 - E_1$~~ 270

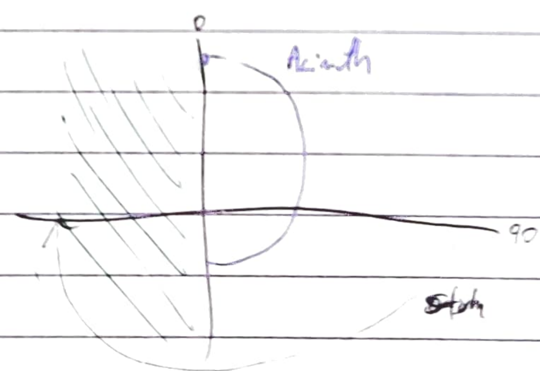
Perhaps really other way?

~~90, 180~~

$270 - E$

$0 - 90 = E_1$

Treat rotation as clockwise



11 APR 2021

Schmid law / criterion / factor

- Describes the slip plane and slip direction of a stressed material which can resolve the most shear stress

Critically resolved shear stress, τ

$$\tau = m\sigma$$

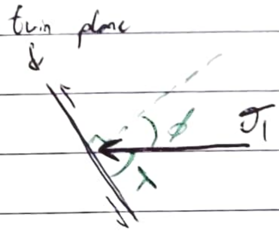
Schmid factor (for m) · Stress applied (for σ)

$$m = \cos(\phi)\ \cos(\lambda)$$

$\phi \rightarrow$ Angle between vector to glide plane & σ_1

$\lambda \rightarrow$ Angle between glide direction and σ_1

Max is at $45°$ because $(\cos 45°)^2 = 0.5$



11 APR 2021

Critical Resolved shear stress (CRSS)

- Component of shear slip resolved in the direction of slip, necessary to initiate slip

$$\tau_{RSS} = \sigma m = \sigma(\cos\phi \cos\lambda)$$

← Schmid factor

Schmid good for single crystals. For polycrystals

Mentions σ here is tensile, perhaps engineering convention!

Taylor G.I. → 5 slip systems

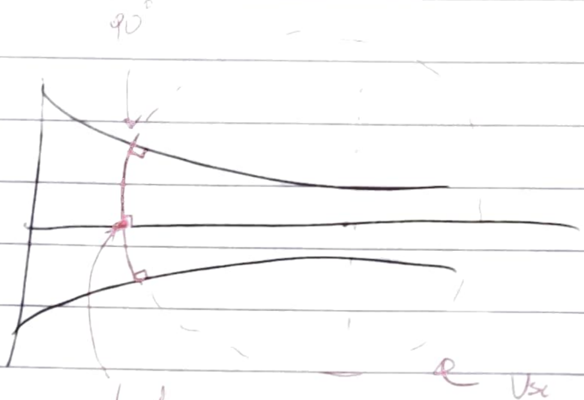
Schmid factor as proxy for orientation

Hmm. Okay

Ernie's 89 Spherical approx paper 11 APR 2021

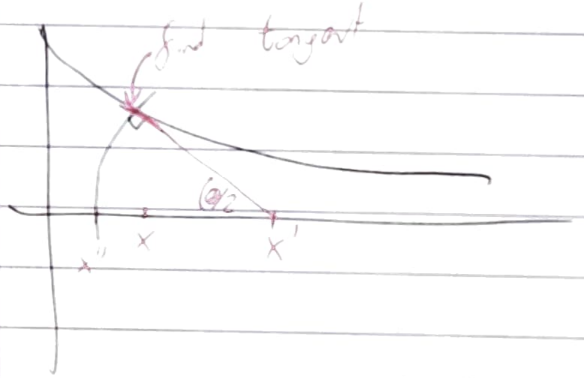
As σ_1 increases, so does σ_m

Solid angle → Ω



← Use solid angle for Area

Working:



1. Describe the sample shape As $y = f(x)$
2. find tangent equation (differentiate) at x
3. find intercept with x-axis (x')
4. find length of this line (sphere radius)
5. $x'' = x' - (4)$
6. Find ~~angle~~ angle with x-axis $(\theta/2)$
7. Find the area subtended ~~a~~ solid angle first

For a cone:

$\Omega = 4\pi \sin^2\left(\frac{\theta}{2}\right)$

Area of sphere $= A = \frac{4}{3}\pi r^2$

To find cone cap area:

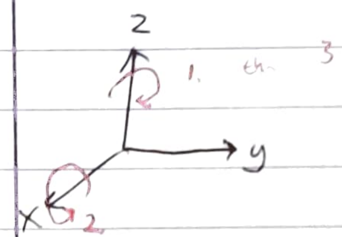
$\frac{\Omega}{4\pi} \times A \quad \Big\} \quad \frac{\Omega}{\cancel{4\pi}} \times \cancel{4\pi} r^2 = \Omega r^2$

12 APR 2021

Look through Euler angle document

Three Euler angles ~~ϕ_2~~ ϕ_1 Ψ ϕ_2

1) Rotation of ϕ_1 about the z-Axis
2) Rotation of Ψ about the rotated x-axis
3) Rotation of ϕ_2 about the rotated z-axis



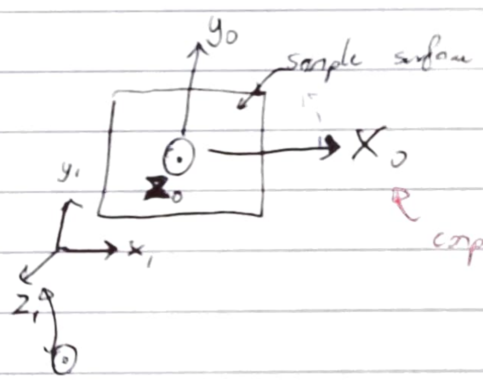
Right hand rule

Not for Z

~~Anticlockwise~~ Clockwise for both WHT

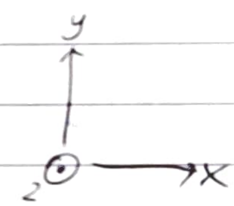
Plot upper hemisphere

Relation to Sample:



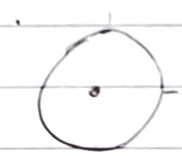
compression direction

And frame is also



Long-Axis parallel to X

001 plots as



On lower hemisphere

ad reference frame, X-Axis is compression direction

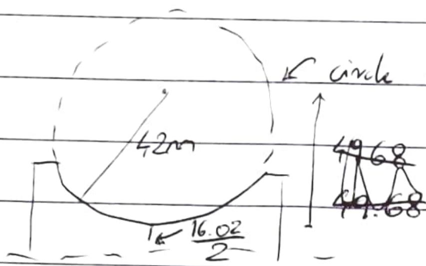
Axis 3-New is c-Axis

c-Axis vertical

A-Axis north

In the end, $\frac{\text{max } \cancel{\text{stress}} \text{ load}}{\text{area}}$ = the pressure

For Geometry



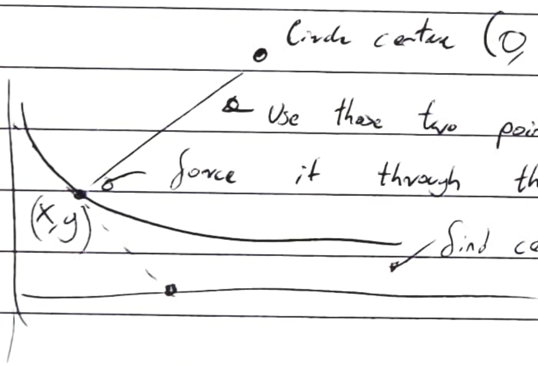
circle of that radius

Circle radius = ~~41.67~~ 42mm

$$(x-a)^2 + (y-b)^2 = r^2$$

$$y = \sqrt{r^2 - (x-a)^2} + b$$

MPa $\cdot$ mm^2 $\qquad (10^6)$ Pa (10^{-6}) m^2



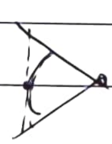
Circle center (0, 50.01)

Use these two points to find equation of a line

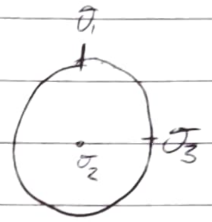
force it through this point, but with $m' = \frac{-1}{m}$

find centre, + find radius

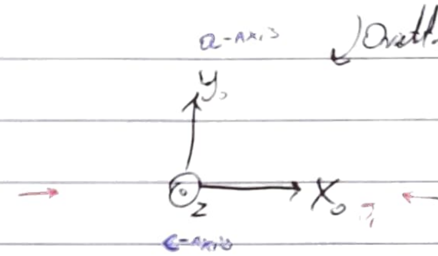
Check Cone opening Angle though



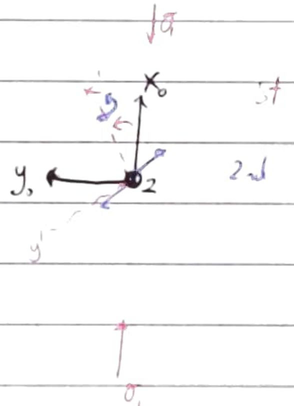
I want a stereonet that looks like:



My axes are such that



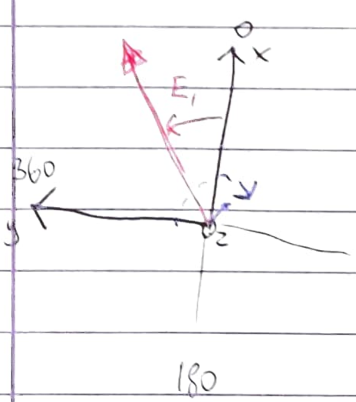
So let's say my coordinates are such that



Upper hemisphere, all rotations +ve

Plunge: if over 90 add 180° to Azimuth ?

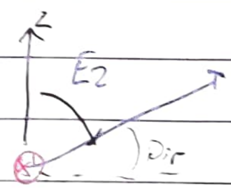
For Azimuth



Azimuth

If 0-90, ~~Strike~~ is +90° from strike

If 90-180, Azimuth is +270° from strike



If less than 90

Dip = 90 - E2

If more than 90

Dip = E_2 - 90

13 APR 2021

Feeb in some points for check:

~~0, 090 should be 090~~

1, 89 should be 089, ~~09~~ 1 ✓

0, 40 should be 090, 50 ✓

95, 30 should be 355, 60 ✓

95, 110 should be 175, 20 ✓

~~110, 110 should be~~

Good I did checks as there were errors (in the code, I think my theory is alright)

15 APR 2021

Selecting best image for Analysis:

- Chameleon montage shows the clearest twins
  ↳ Slightly oversized.

Enrico's Dec 10 email:

USse Euler to work out 3 possible orientations plot that on image, and see which matches → fine?

Work out Euler. Remember vector will be ⊥ to e-plane

But actually if I plot 3D line on 2D image, it should project just right → Or actually plot the plane for z = 0 to ~1 + small range compared to label edit
But best if I find intersects

Jobs for ¿Tuesday? ← Place figure in matlab and coordinate with (0, 0) as origin.

Right-hand side is a bit off-axis, so given coordinates will not work perfectly

20 APR 2021

Direction comes from Plunge/Plunge Azimuth in right-handed system:

θ – Azimuth

δ → Plunge

$\cos\delta \sin\theta = \cos\alpha$

$\cos\delta \sin\theta = \cos\beta$

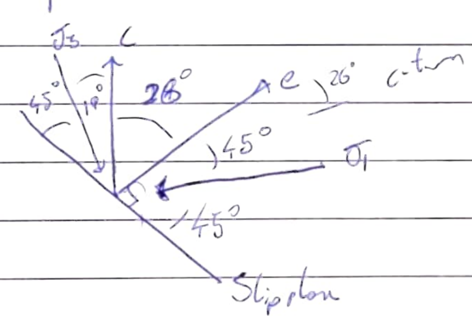
$-\sin\delta = \cos\gamma$

Because I'm using upper hemisphere, I will probably want a negative sign somewhere in this equation

Success! All angles but for Grain 26 are about 52°, as expected

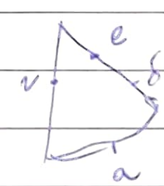
80°

C-E plane



Thought → ~~no a-axis, but probably n~~

actually no. ~~Half is through~~

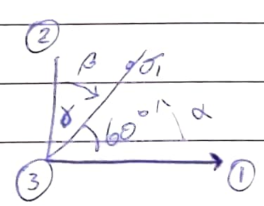


60° slice

The plane containing e is 30 degrees from nearest a-~~plane~~ Axis and 60° from nearest n-Axis

But, it also is 90° from the next A-Axis

Ernie's Diagram:



20 APR 2021

Current thought process →

~~Find direction cosines from 3 euler angles~~

- Find rotation matrix of one ~~p~~ system onto the other
- Establish all angles in system I
- Carry out the rotations

If no success see what Ernie says

Okay. Using even Euler angle of Host, should be able to guess directions of ~~hosts~~ twins, and hence also σ_1.

Can use existing grains as a benchmark here.

Good idea. Application will be non-trivial :(

Why does Ernie use plane 60° from ① ~~a~~-Axis? ~~a~~ m-Axis
Doesn't c lay on m-axis?

First rotation: phi 1 range -180 to 180 about z

Second rotation: theta range 0 to 180 about x

Third rotation: phi 2 range -180 to 180 about z

phi1	theta	phi2
ϕ	θ	ψ
E_1	E_2	E_3
phi	theta	psi or phi2

$$R = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$A_{11} = \cos\boxed{\psi}\cos\boxed{\phi} - \cos\boxed{\theta}\sin\boxed{\phi}\sin\boxed{\psi}$$ E_3

$$A_{12} = \cos\boxed{\psi}\sin\boxed{\phi} + \cos\boxed{\theta}\cos\boxed{\phi}\cdot\sin\boxed{\psi}$$ E_1

$$A_{13} = \sin\boxed{\psi}\sin\boxed{\theta}$$ E_2

$$A_{21} = -\sin\boxed{\psi}\cos\boxed{\phi} - \cos\boxed{\theta}\sin\boxed{\phi}\cos\boxed{\psi}$$

$$A_{22} = -\sin\boxed{\psi}\sin\boxed{\phi} + \cos\boxed{\theta}\cos\boxed{\phi}\cos\boxed{\psi}$$

$$A_{23} = \cos\boxed{\psi}\sin\boxed{\theta}$$

$$A_{31} = \sin\boxed{\theta}\sin\boxed{\phi}$$

$$A_{32} = -\sin\boxed{\theta}\cos\boxed{\phi}$$

$$A_{33} = \cos\boxed{\theta}$$

Do it and do trial and error

Input:

0,0,0

Expected output? ✓

	x	y	z
v_1	1	0	0
v_2	0	1	0
v_3	0	0	1

x-Axis points towards x ✓

y-Axis points towards y ✓

z-Axis points towards z ✓

90,0,0 ✓

Success.

Figured out how Ernie's 'corrections' work for stereonets but I don't think I need them. → Actually removes potential symmetry errors

21 APR 2021

If I do all three Euler direction cosines:

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{array}{l} n\text{-Axis} \perp \text{to } c \\ \leftarrow a\text{-Axis} \perp \text{to } c \\ \leftarrow c\text{-Axis} \end{array}$$

Look up Rodrigues rotation formula

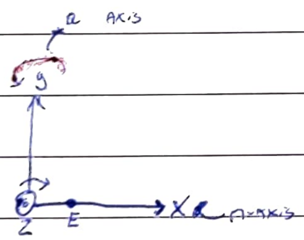
$$\underline{V}_{rot} = \underline{V}\cos\theta + (\underline{k} \times \underline{v})\sin\theta + \underline{k}(\underline{k}\cdot\underline{v})(1-\cos\theta)$$

→ uses right hand rule

$\underline{K}$ is the unit vector describing rotation Axis

$\underline{V}$ is the vector that will rotate

θ is the angle of rotation



So, c-Axis, or $\underline{z}$ is the $\underline{v}$

a-Axis, or $\underline{y}$ is the $\underline{k}$

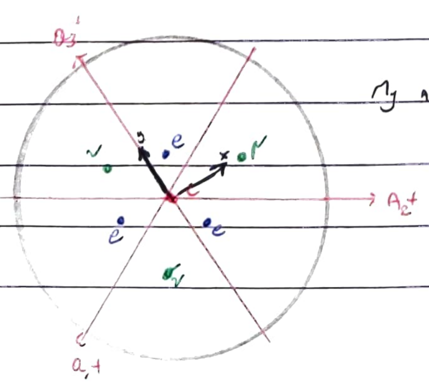
Going from $\underline{z}$ to a is in positive sense.

(However machine conventions may be a problem?)

Going 26° gets me to ~~a~~ Actually, at +a, this gets me to a v plane.

* Will probably get me to a point 60° off the a-axis, so below

Either way, solution can be shifted about. Add 60° to go from v to e containing n-plane → around z-Axis of course



my axes h.t v

Apply it! ← try finding this explicitly first to confirm:

1. Rotate around y by 52°
2. Rotate around z by 60° if necessary

But first get the angles to direction cosines...

Success!!

22 APR 2021

Confirmed that it is possible to rotate the Measured host into an Orientation that corresponds with the measured twin.

This involves, as previously stated:

1. Rotate by 52° around y(a) axis so that $z \rightarrow z'$
2. Rotate z' by 60° around z so that it hits the c-e plane $\rightarrow z''$
3. Further rotate by 0°, 120°, or 240° to index with 1 of 3 symmetries.

Usually z'' is within 2° (sometimes up to 10°) from measured value.

Next task: Convert direction cosines to azimuth/plunge so they can be put on stereonets.

Potential equations:

$\theta = \mathrm{Atan}(\cos\alpha / \cos\beta)$ ← 0-90, must do quadrant analysis

$\delta = \mathrm{Asin}(-\cos\gamma)$ ← Once again cosine negative for upper hemisphere.

Or even -1cos δ to deal with symmetries

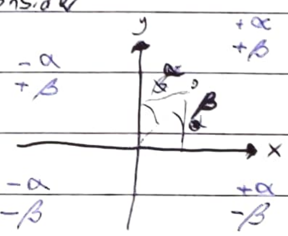
Actually may need to change signs of ALL direction cosines

Azimuth	$\cos\alpha$	$\cos\beta$	θ
0-90	+	+	θ ✓
90-180	+	−	$180+\theta$ +
180-270	−	−	$180+\theta$ +
270-360	−	+	$360+\theta$ +

Questionable

All correct ✓

Consider:



Success!!

Cosine-to-Azimuth works well, and in a predictable fashion

Next: Plot σ_1, e plane, and σ_3 for known pairs

22 APR 2021

For Signal finding

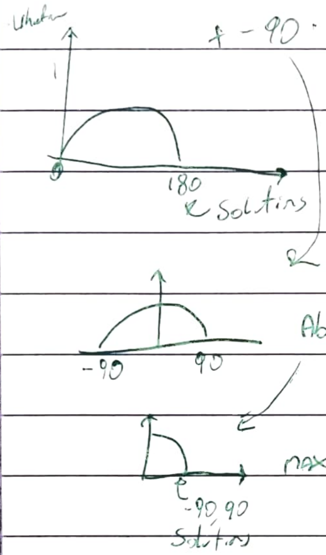
I need to select when $\Delta\theta$ is close to 0° or 180°

& Actually think about implications. Is it better to rotate it around?

Test this

Grains: 90, 163, 292, 311

To find value closest to 0 or 180



will give solution

In this case:

y-Axis aligns

Rotate by 180° around y? Is it necessary?

See what starcomet does

Grain 135 is problematic → because 10° between estimate & actual twin c-Axis

Maybe write a function that will write tables with Headers, otherwise ~~we~~ the text files may get confusing

Tomorrow try to plot extension direction

23 APR 2021

Proposed method for plotting on traces of e-planes and v-planes

Once pole to a plane is found, $\hat{p}$, we want the trace of the plane it represents, as it intersects the x-y plane.

This trace is perpendicular to the pole $\hat{p}$.
This plane is also always perpendicular to the z-axis.
(x,y)

~~in geographic reference~~
(0,0,0) Euler

Here, do cross-product $\hat{p} \times \hat{z}$ to get the direction of the trace. → which should have only (x,y) components

Because $\hat{z}$ is not always perpendicular to $\hat{z}$, output is not a unit vector, and will need to be normalised.

Then do necessary adjustments (lengthen vector) so it shows up well when overlaid on the image

Should work. Task for next day
- Reuse lots of signal code probably
→ + first ~~@~~ test on known grains

27 APR 2021

Poles to cleavage planes are 44° from c

Establish E-plane and R-plane poles for all grains

Cleavage plane: May be confusing it with twin plane
63.9 (or 26.1°) according to 2016 paper

Note from Miller-Bravais indices: [0001] are direction of poles to planes
(0001) are planes
<0001> are families of directions ✓
{0001} are families of planes

Spiers 1980 → 44.5° for c-r
Emine confirms 44° in email

Try to confirm this using:

$\cos\phi =$ Actually dead end :/

Try inputting indices as $[h\ k\ i\ \frac{3}{2}(a/c)^2\ l]$, which should be a normal.
$a = 10$
$c = 8.5$

$[h\ k\ i\ l]$ factor = 0.922 → pointless :/

$i = -(h+k)$
unnecessary

Directions represented by uvtw
need all 4

e is $(\bar{1}018)$ $\langle 40\bar{4}1 \rangle$
r is $(10\bar{1}4)$ $\langle \bar{2}021 \rangle$
c is [0001]
f is $[\bar{1}012]$ $\langle 2\bar{2}01 \rangle$

28 APR 2021

Plotting of traces figured out - now must worry about comparing results to image

Grains 8 and 198 are the least misoriented (6 & 8° from geographic z-axis respectively.

Everything else seems to work fine

For some grains, like 19 or 53, the e_1 / e_2 traces don't really line up - maybe 10° mismatch. The closest solution however is the one picked up by the EBSD

Change of tactic: Instead of trying to plot the traces on top of the image in Matlab, try to do it in illustrator. There are some advantages to this:

1. No axis mismatch to worry about
2. No grain coordinates to worry about
3. Easier to adjust size as needed
4. Easier to shift about as needed

→ However add grain number to axes so it is clear what I am talking about

I AM AN IDIOT!

- Everything is fine. I didn't set up the chart dimensions right, so they came out a bit "squashed". After correction everything is okay. x/y lim [-1 1] pbaspect [1 1 1]

↳ Anyways, proceed with this

28 APR 2021

Success! Generated 322 images (for each grain)
Need to overlay them on channeling image now, and collect twins → solutions
in a seperate spreadsheet

Grains that can't really be analysed:
6 - v overlaps the only e(3)
7 - Grain doesn't really exist on channeling
10 - Two ~~v-axes~~ planes on prominent e(2) - exactly
15 - No twins, but it's small and fractured so inconclusive
18 - e(2), but small miss-match ~10°
22 - e(2) possibly overlapped by (v)

F-slip analysis successful from grain 16

Δ
└ Created A word document for these probably a better route

204 - perfect grain :)

30 APR 2021

Good unique unambiguous solutions

17 & 19 are the same grain → good example of Δ our limitations.

01 MAY 2021

Convert from Direction cosines to Euler angles.
- Important as will make using older code 10x easier

$a_{31} = \sin\theta_2$ ← E_2

$a_{32}\cos\theta_1 = -a_{33}\sin\theta_1$

$\frac{a_{32}}{-a_{33}} = \frac{\sin\theta_1}{\cos\theta_1} = \tan\theta_1$ Here: $\theta_1 = \text{atan}\left(\frac{a_{32}}{-a_{33}}\right)$ ← E_1

Actually think this is a different convention. May come back to it later. Try from 1st principles:

E_1 E_2 E_3
ϕ θ ψ

Worry about +/- solutions?

$a_{33} = \cos\theta$ $\theta = \text{acos}(a_{33})$ E2 solved ✓ θ known

$a_{31} = \sin\theta\sin\phi$ $\text{asin}\left(\frac{a_{31}}{\sin\theta}\right) = \phi$ ~~E_1 solved ✓ ϕ known~~

$a_{13} = \sin\psi\sin\theta$ $\text{asin}\left(\frac{a_{13}}{\sin\theta}\right) = \psi$ E_3 solved ✓ know ψ

↳ Doesn't quite work. Unsurprisingly

Problematic when E_1 is over 90° !!

Better Solution: Someone already wrote good (excellent) code for this that takes account of all orientations and zeros ($1/0 \to \infty$ problems)
↳ Adapted that and it works perfectly!

02 MAY 2021

Objective:
Write code that will "summarise" the twins from ANY file, provided grain No. is in the first column.

What is means is: Removes problematic grain rows, using problematic grain "key".

This will make the tables of data less troublesome when feeding into other code.

Complete:

Now try to get Sigma1 and Sigma3 onto stereonet

Note: "Extract-Correct" software/code will do rotations to Sigma1 and Sigma3 when minorly adjusted

Imp: run "Extract correct" and "Prepare for Stereonet" together

To generate poles/vectors

To remove problematic and prepare for plotting

If need something in Cone: Run "Extract correct" to generate Eulers. Then run "Remove_Problemat..".
Then use parts of "Prepare for stereonets" to summarise if needed

perhaps best Not to do it yet, as it will be easier to append pressures, durations etc to "untouched" data - where row 1 = Grain 1

Perhaps add this to "Extract correct"

NO → will mess up the part

Catch up on work →

Inverse pole figure first.

- Start by doing a inverse-order negative sense Euler rotations. (That will tell you how to get the crystal back to geographic axes. In cosine terms, x-axis is the signal!)

See where it gets data. Rotate by 120° around [001] crystallographic if needed (if-statement)

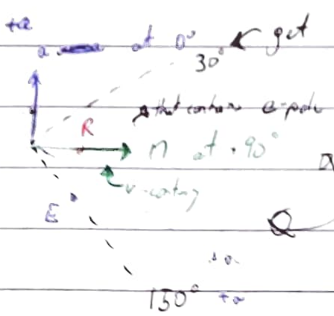
Try this. Then try this for a-poles. → from Euler. See where it goes.

Add inverse pole Euler to code list

Seems to work! Nice!

Split up based on twin no. and remove problematic

As it stands:



← get everything into this state

that contains a-pole

v-coating

~~Actua~~

Q — then reflect about c to get bottom bit

Problem → If A at is -ve, I might have rotated in RE by accident

Think about this again tomorrow as it is wrong

For Schmid factor:

Do this for a list of non-problematic E-planes

$$n = \cos(\phi)\cos(\lambda)$$

ϕ ← Angle between e-pole and σ_1

from Extract Correct ~26° on CE plane

[100] ← Always x-parallel

λ ← Angle between Slip vector

~64°

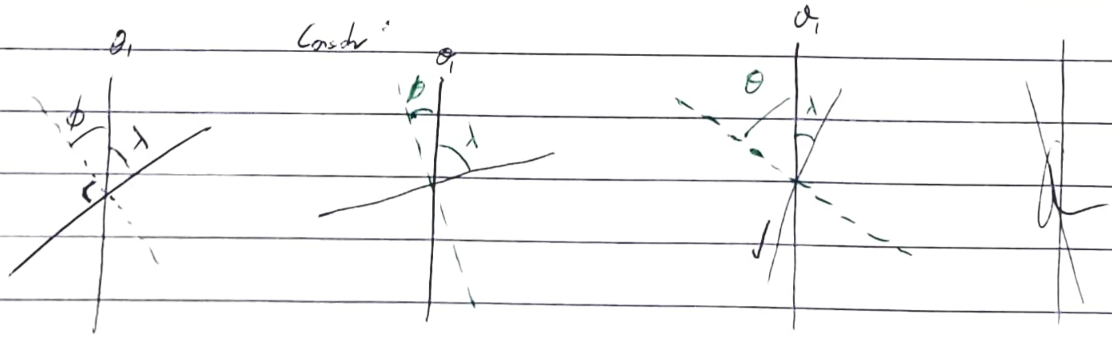
Along CE plane

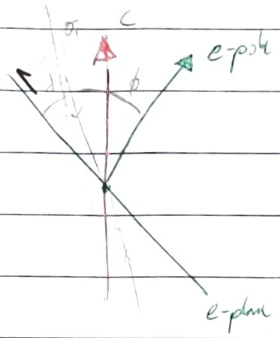
Only 64 twins with positive Schmid factor

And they also plot right in the middle of the stereonet. Probably got exactly the wrong ones

Actually, by definition, maybe negative are in fact meant to be solutions:

Consider:





I think λ should be the ~~angle 90~~ $180°$ - angle between vectors, as that then finds the actual angle to the slip vector

Now 182 good twins

~~F poles: 150,~~

For great circles to do Spiers twin-zone plot.
Either λ or ϕ must $= 90$ for zero resolved stress.

So poles are e-poles & slip vectors

e-poles:

150, 26
30, 26
270, 26 ← Rember upper hemisphere, & it work great

slips:
330, 64
210, 64
90, 64

05 MAY 2021

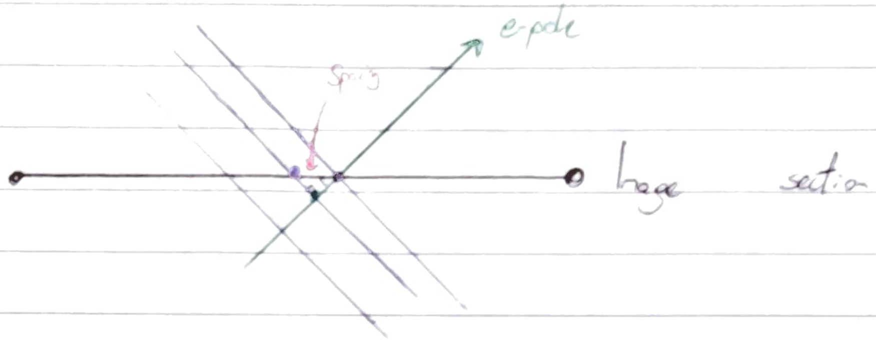
Add to problematic list:

181 – Actual solutions are 3 and 2 - I must have made a mistake earlier

283 - Same story → Actual solutions are 2 and 3

Actually fixed that → It will need to generate figures again → And check if Schmid factor is still good.

Finding the twin density ↷ Corrected for image section effects



$$\text{Density} = \frac{\text{Number of twin planes}}{\text{Grain diameter}} \quad \text{twins/mm}$$

$$\text{Spacing} = {}^{1}\!/\,\text{Density} \quad \text{mm/twin}$$

Show histogram of dips

$$\cos\theta = \frac{\text{adj}}{\text{hyp}}$$

$$\cos\theta = \frac{\text{corrected spacing}}{\text{apparent spacing}}$$

$$(\text{apparent spacing})(\cos\theta) = (\text{corrected spacing})$$

$$\frac{1}{(\text{apparent density})}(\cos\theta) = \frac{1}{\text{corrected density}}$$

$$\boxed{\frac{\text{apparent density}}{\cos\theta} = \text{corrected density}}$$

◦ Goal - find dip of e-pole for all sections now.

All done ✓

09 MAY 2021

Tasks for today:

- Extract a list of good grains + twins + diameter + pressure from the massive spreadsheet.
- Sort them into ~~3~~ size categories.
  ← Maybe more - will see
  [0-50, 50-100, All above 100]

☑ • Plot twin activity against Schmid factor ← Not very fruitful
☐ • Twin activity against Pressure ← Not very fruitful

Then further divide into groups by Schmid factor and plot:

☐ - Twin activity against Pressure for each Schmid group

Matlab storage format:

10 MAY 2021

1	2	3	4	5
Grain	Schmid	Twin Activity	Diameter	Diff pressure

1st

Grain size →

Schmid ↓	0-50	50-100	>100
<0.2	1 — 8	2 — 22	3 — 31
0.2 - 0.4	4 — 10	5 — 21	6 — 45
0.4 - 0.5	7 — 7	8 — 18	9 — 20

2nd

Do same for Schmid factor vs A

Grain size →

Pressure	0-50	50-100	>100
<340	9	16	37
340-360	7	19	22
>360	9	26	37

A

3rd P-plot Size 50 - 150 um

~~165~~

285 — 5 (295)	295 — 2 (305)	305 — 4 (315)
315 — 7 (325)	325 — 4 (335)	335 — 6 (345)
345 — 17 (355)	355 — 27 (365)	365 — 33 (375)

10 MAY 2021

Gradient of Schmid / Activity may be related to pressure

→ Smaller pressure = Bigger gradient

Try plotting Activity/Schmid vs Pressure → Should see a positive relationship

Still try this in grain-size graphs

Thesis Structure Document

11 MAY 2021

Thesis Layout:

Introduction

- Explain the term palaeopiezometry
- Explain Calcite (briefly) and how it makes marble rocks - including Carrara Marble. → Show some "habit" diagrams. "Clinographic projections"
- Describe twinning - both growth and deformation
- Explain the basis of "Experimental calibration".
- Briefly introduce my approach - how thanks to EBSD I will now be able to use orientations. And how current methods are 30 MPa Limited.

Background:

- Work by Ernie in 80s/90s - all the dependencies
- Importance in lower crust
- Weiss from 50s
- Spiers
- Karakoram from 07 + other potential applications.

Experimental set-up and data collection

- Drawing, numbers, etc. → Strain/pressures, time
- Dog bone shape
- Sample cut in half and EBSD'd by dave wallis

Data generated:

- EBSD Map, + Orientation data (Explain EBSD + reference) → Explain Euler Angles + Bunge notation
  - For hosts and some twins
  - + Grain Area
- Channeling image
- Band contrast image

e ①

Theory: Orientation Theory

- Start with Objective: To use ~~information~~ Orientation information
Basically (Part I)

11 MAY 2021

Grain size and pressure Theory:
- How grain size is worked out (feret diameter)
- How pressure is worked out (Part 2)

Analysis (Orientation)

- Start by analysing orientation of c-axes, E-poles and angles between them. (Show how Euler → Cosines in Bunge convention) Mention ↑ formulas
- How other orientations are worked out. Mention Rodrigues rotation, how CE-axis is 60° off CR-axis, and how there are three solutions.
- Turner Weiss on known grains. Mention problematic 135 + 26.
← This is a confirmation, but show 30° offset - comment how this may be a pre-existing fabric
- THEN how 3 solutions for each were generated. (as e-poles) These e-poles were transformed into traces by x-product with sample z-axis. ← This gives traces. Give some examples.

- Those are overlain on image and solutions recorded. Show some perfect and some commonly problematic grains. Mention stats. How many of the 323 grains are good, how many poles, etc.

- Do ~~T~~ ~~Sch~~ Turner-Weiss analysis with these → This will still be problematic cause of negative Schmid factor.

- Do Schmid factor corrections → Then Turner Weiss again

- Explain how inverse pole figures are generated, and do one for (0, 1, 2, 3 twin zones)
~ Spiers

- Counting twins and e-normal corrections

11 MAY 2021

Grain size and Pressure thgs here
- Grain size as Feret diameter

· Pressure by spheroid shell approx, as shear stress at sample surface must = 0
 - Show some pressure - distance graphs.

LINKING PRESSURE WITH TWINNING
· Showcase the graphs and explore potential correlations,
-Explain why it's important to split into grain-size groups.
↳ Explore splitting into Schmid factor groups
↳ Add the one last resolved Shear stress bit if time permits

Rename Pressure to whatever it is Ernie called it

Discussion:
What's in the word file ↗ A lot more twin planes collected
Discuss some more errors:
- Bigger sample vs grain size - propose further studies with mock of different grain-size distributions
· Potentially some planes identified as twins are NOT twins but slip on non-v, non-S planes that overlaps. ↖ Also pre-existing
Discuss Neighbour effect
- Suggest further manipulation of the data

Conclusions:
- Tomar Weiss Analysis Works great
- Zones predicted by Spiers generally seen
· A LOT More twin planes available to study thanks to trace method
- Further analysis of transformed data (as in Erkin's email)

Acknowledgements: Like in Word file

WORK:

27 MAY 2021

① Presentation plan

Intro
→ Define terms
→ Why it's useful
→ Calcite geometry
→ Data available → Why calcite is useful
→ Snapshot of analysis

- Define Palaeopiezometry ①
1. Introduce the concept of measuring pressure at depth
   - Like with metamorphic paragenesis analysis.

2. Define differential stress.

3. Explain the utility of a piezometer → Can tell stress state in Wells, but also study of Regional tectonics
   → in 2007 a shear zone was defined thanks to Calcite palaeopiezometry

4. Intro into calcite → Start very basic.
   → Made of calcium Carbonate → Main constituent of marbles

5. Calcite structure → Rhombohedron
   - What's important is that it has three a-axes, and optical c-axis.
   All a-axes are identical, but are of different length to c-axis ← this varies with temperature thanks Paul & Steve.
   Going back, the importance is symmetry.
   There is reflection and inversion symmetry in Calcite too, but all we care about is rotation, as all our action happens right on the mirror-planes. Stereonet * Write that it's upper hemisphere

6. Step back to twinning - Definition (reference)

7. ~~We require Twinning can happen~~ on three Twinning we are interested in is called the e-plane twin, because it occurs on e-planes
   Point it out
   - E poles

(2)

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8 - $\boxed{\text{Show where a-plane is on calcite,}}$ but mention this isn't important. What is important is that it lies on a mirror-plane, ~~50 degrees~~ 26 degrees away from the c-axis and there are 3 of them

9. ~~Show angle~~ ~~M~~ Switch topic to Resolved shear stress
! Show the equation of schmid but don't call it that yet !

Explain what the terms mean in 2D

Show a plot of cos θ × sin θ to show a max of 0.5 when θ = 45°.

I.E. Resolved shear stress largest when stress vector is at 45°.
→ Called "Schmid Factor"

10. Now sum it all up : e And applies in 3D as well
$\boxed{\text{Show Angle relation}}$
- Sigma 1 at 71°, 26 + 45° from Host, towards E-pole.

- Note that in calcite there can be more than one active slip system - Question

! This forms a basis of one analysis performed. If we assume all the twins are optimally oriented, and signal is at 45° from the twin plane, and we plot ~~this~~ signal 1 estimates for multiple grains, we shall know where the actual sigma 1 is.

Turner - Weiss

11. This is what this graph shows. Of course ~~almost~~ none of the grains will be ~~too~~ perfectly oriented, hence we have a spread. But after contouring, ~~we~~ we see that the prediction is spot-on. North and South poles are the actual ~~point where~~ ~~Sd~~ stress directions

(3) Channeling image fragment without traces 27 MAY 2021

12. ~~But how did~~ But that's part of data analysis. First we had to gather all this data.

I won't have the time to ~~pass~~ showcase all the data I was presented with, but let me show you the most essential parts.

[Channeling image - Something in the corner]

This is ~~actual~~ an image which shows ~~a slip systems~~ traces of many ~~slip syst~~ slip systems. Some of them will be e-twins, and some will not.

· We also know the orientation of each host grain. This isn't shown on the image - it's part of numerical data generated by the EBSD

13. Traces appear Remember, the geometry we learned about before, through some complex math we can predict ~~those~~ ~~the twins will fall~~ what the expected trace of each plane should be. This is shown as the coloured lines on the graph.

Essentially, by analysing this image, which contains over 300 grains, but we only see a handful on the screen now

14. Table with no of twins collected

This method allowed for collection of 216 twin planes but after filtering of problematic data this number dropped to 152 [? Ask why so many grains were ~~rejected~~ filtered off]

This is a ~~@@~~ 700% improvement on ~~what the~~ the volume of data that EBSD has collected

[List of things]

27 MAY 2021

Ⓒ

15: To finish off, few details why we might want to look into it further: [Locate]

- Research has shown that it is Temperature insensitive*
  Pressure ins. Strain-rate insensitive
  Good things

~~Hence can tell pressure at~~ ~~Grain size~~ Grain-size sensitive
  ~~Needs more work~~

16. ~~N~~

Stress magnitude graph → I tried using new data, but it requires more work. I think ~~the~~ I may have more success if I re-evaluate ~~~~ how I define and measure twinning activity.

~~17. Comments~~
~~17. Qs?~~

But that's all we have time for today. Any Qs?

17. QS?

18. Reform