Reviewer's comments on "Texture analysis of experimentally deformed Black Hills Quartzite" by Rüdiger Kilian and Renée Heilbronner. Submitted to Solid Earth.
Review by Dave Prior, University of Otago

Apologies for being slow in reviewing.

This paper has the potential to make an excellent contribution to our understanding of quartz deformation. The paper presents a high quality EBSD data set from some experimentally sheared quartzites. The data are used to demonstrate that there is a transition in crystallographic preferred orientations (CPO) as a function of different deformation conditions. In a high stress magnitude experiment [c] axes are clustered around a direction rotated a few degrees away from the normal to the shear plane. In a low stress experiment the [c] axes are clustered in the shear plane normal to the shear direction. The microstructures of these experiments correspond to recrystallisation regimes 1 (high stress) and 3 (low stress) as defined by (Hirth and Tullis, 1992). CPOs from a regime 2 (intermediate stress) sample are transitional. The authors use the EBSD data to relate closely the CPO and the sample microstructure to with the aim of providing a more robust understanding of CPO forming processes. The authors argue that long held ideas of the transition they describe being related to changes in dominant slip system as a function of increasing temperature are not consistent with the new data. One key interpretive outcome is that basal <a> is not an important slip system in quartz deformation. If this is demonstrable, it is really important and upsets conventional thinking. This work has specific importance to researchers using quartz microstructures to understand crustal tectonics and more general importance to researchers with an interest in deformation microstructures.

Although I think this is an important paper, it needs major modifications to ensure that it has appropriate impact. In its current form it will be ignored and very few will understand it. At present it is way too long and it's a really hard read. It needs to be rewritten so that it is easier to understand by both a general audience and by microstructural specialists. I consider myself a microstructural specialist and there are large parts of the manuscript that are completely indecipherable. There are sophisticated analyses that do not really contribute to the paper's key conclusions and these need to be reduced or removed to focus on the key new information. The discussion and conclusions do not build upon the observations in a logical way that is easy to follow. A much shorter more focussed discussion will be much more effective. I think that it is possible to reduce the paper to a much better paper of one third to one half the current length. The paper is sufficiently unclear that I cannot really judge the robustness of the interpretations. The paper needs to make its case with considerably more clarity.

Below I outline some scientific points I think the authors should address and a set of recommendations on how to make this paper much more accessible. What I've written here is a mere subset of more extensive comments on an annotated .pdf file of the manuscript. In is important to bear in mind that Solid Earth is a broad journal and it is important that geophysicists, petrologists etc read this paper and understand it. In it's current form they will likely not read it and will find it very difficult to understand.

Scientific comments.

i. *CPOs a function of stress.* The authors argue that the three samples are all deformed at about the same temperature and at the same strain rate and that therefore the stress is the key difference between the samples. Although I agree that for these experiments stress is the parameter that changes the most, I do not think that allows you to argue that temperature or strain rate cannot also be parameters that will affect the microstructures. (Hirth and Tullis, 1992) relate the three regimes to both temperature and strain rate and could equally well have related them to stress. Furthermore you need to explain why the stresses are different in the three samples. The quartzite behaviour will be described by some composite flow law, so changing stress in isolation is highly unlikely; different strain-rate, T, or water content must control this. Although the temperatures are argued to be almost the same, the change in temperatures across the three samples is consistent with the changes in stress (lower T gives higher stress). If I plot a log stress vs 1/T Arhenius type plot using the flow stresses I get a straight line for all three points although the activation enthalpy I calculate from this (760kJ/mol) is much higher than literature values (Hirth et al., 2001). This makes me wonder whether anything else is changing. The key candidate for me is strain rate. The authors say the samples are all deformed at the same rate. The rate is quoted in the methods as the axial shortening rate*, which I would presume is that measured from piston displacements during the experiments. Given that these are general shear experiments I think it's highly unlikely the rates are the same for all experiments. Indeed the table in the companion paper lists them as different. My conclusion is that the flow stresses you have are the function of T and strain rate variations between the samples. The authors make some comments on the role of water from line 592 (too late in paper). Maybe water content differences explain the stress differences (although two samples are listed as the same water added?). Even if this is the case arguing stress as the only parameter is naïve.

* note: I cannot make sense of the strain rates. I don't know where sample w1092 is from. It is not used in either of the Heilbronner & Tullis papers quoted. w935 is assigned a shear strain rate of $2*10^{-5}s^{-1}$ by Heilbronner and Tullis 2006 and the methods say that an axial shortening rate of $1.2*10^{-6}s^{-1}$ was used. For the same sample (and for w946) Heilbronner and Tullis 2002 provides a shear strain rate of $3*10^{-5}s^{-1}$ (as used in this manuscript). I've just looked at table one in the companion manuscript (H&T 2017- that gives a range of shear strain rates for each of the three samples and they are not the same. It's not very good if two papers on the same samples in the same journal and year have different values for strain rate! I'm sure there is an explanation- important to sort this out.

ii. *Lack of strain series*. The three samples are all deformed to about the same strain and probably along different mechanical and microstructural pathways. The strain series has two points each (undeformed and deformed) on three pathways. In this case, the coincidence of CPO components (e.g. Y maximum) with particular microstructures (e.g. high intragranular strain) is not documentation of a kinematic model (e.g. rotation of c-axes from the periphery). Similarly changes from regime 1 to regime 3 are not representative of a strain series. It's not robust to make interpretations of CPO evolution from your data alone. The discussion of kinematic models needs to bring in the evidence from experiments or natural samples where a strain/ time series is reasonable (e.g. (Cross et al., 2017; Heilbronner and Tullis, 2006) from experiments, several papers from natural examples).

iii. *<a> axis alignment.* I really like the idea of using the intergrain <a> axis alignment (fig 8). I think this general approach could be very useful in other systems (ice in particular). I have a gut feeling that something useful can come from this analysis for this paper. However, at present the use of these data fall into the class of "fancy analysis that goes nowhere" in point 6 below. Part of the problem maybe that you show this only for the regime 3 sample. All the other key points in this paper come from comparison of the three samples and I think this is necessary to show the value of the <a> axis alignment. For example is the pattern shown in fig A2 the same in all three regimes? I think that a key point that may come from fig 8 is that the Y domains provide greater volumes (larger domains?) that can deform by <a> slip? The figure does not really show this well. I wondered whether it would be useful to show a map where domains connected by thresholds in <a>transparency are shown (and coloured as Y, B or other). This approach has some similarities to the grain boundary hierarchy approach (Trimby et al., 1998). Such data for the three regimes may show key differences in size and connectivity of <a>transparent domains. These observations may then be linked to the interpretations about slip system activity.

iv. *Lots more-* see pdf.

Making this paper more accessible and understandable.

1. *Abandon "Texture".* Throughout this paper the term "texture" is used with the meaning common in metallurgy and materials science. There is a very small community of geoscientists who use "texture" in this way. For the vast majority of the geoscience community "texture" means the spatial relationships of phases and microstructures. To most geoscientists texture is what you would see down a microscope (in a petrographic examination for example) and is broadly synonymous with the term microstructure. Textbooks in geoscience use the term texture in this way and there are specialised textbooks on textures that take this meaning (Metamorphic:, Barker, Shelley. Spry, Yardley & Mackenzie. Igneous Mackenzie & Mackenzie, McPhie et al., . Sedimentary: Holt, Scolle. Ore Minerals: Edwards, Taylor). I did a web of science search for "texture" in the title and "rock*" in the topic. This recovers 888 papers. All but 4 of the newest 50, all but 2 of the oldest 50 and all but 3 of the highest-cited 50 use texture in the geoscience way rather than the metallurgical way (I've no time to look at 888). Having "texture" in the title is particularly problematic as most geologists/ petrologists will misinterpret it and most geophysicists won't know what it is. The terms "crystallographic preferred orientation" (CPO) or "lattice preferred orientation" (LPO) are much better as they are explicit. If you want this paper (and the companion paper) to have wider readership, remove the word texture throughout and replace with CPO or LPO.

2. *A diagram to explain your reference frames.* The names used for various orientations of c-axes on the pole figures are explained in words around lines 80-93. This is not very satisfactory: these need to be shown in a figure. A figure will act as a constant point of reference for readers looking at the results or discussion and trying to remember what particular grains or domains are. Remember also that most of Solid Earth readers will be unfamiliar with the general shear kinematics. Many will be unfamiliar with pole figures and especially with inverse pole figures. So a simple figure that has:
    a. A cartoon of the general shear geometry and kinematics (like lower part of fig 1c in H&T, 2002)
    b. A stereonet to show the various "domain" and "grain" orientations used in to describe the CPOs and the angle conventions (where domains relate to variable angles). Some key directions should be highlighted on a.
    c. An IPF as used later in figs to show key crystal directions used.
    d. This figure could also be used to relate names used in this paper to alternative names used in the literature – reducing text length and making these links clearer.

    This figure will make the paper much easier to understand and will enable some of the figs that follow to be simplified.
3. *Crystal axes.* On lines 126-128 the indices and names of crystal axes are related. In the rest of the paper these two forms are interchanged. For example most of the figs use the indices and most of the text the names. This makes it difficult to read for those not familiar with indices in the trigonal system. I would stick to the names ([c], <a> etc). The words you have (l126-128) are still needs but then stick to names in text and figs.
4. *One point per grain vs one point per pixel.* There are valid reasons to explore which of these choices are made. The complications added by showing a mixture of both makes this paper harder to follow. The choice makes no significant difference in any of the data presented (this is said somewhere but can't find it) so just pick one way. This will shorten the text and reduce the size/ number of figures. I would pick one point per pixel (all orientations).
5. *IPF ref frame choice.* A mixture of extended and folded IPF forms are used. I'm sure there is an argument as to which is used where, but this is another thing that will act as a significant point of confusion. On figs 2b and 8b I can see that it is important to have the folded form. In none of the other figures does it matter. The IPFs in fig 1b are mostly symmetric and little useful information is lost in folding them (also inconsistent to show these in extended form and not <a> pole figs on whole sphere). Actually I don't think there is any information in the IPFs in Fig 1 that you don't get from the pole figs. So why not just remove them. I would switch to folded IPF throughout and also make the colour schemes of IPF s the same (e.g figs 2a,b and 8b).
6. *Fancy analysis that goes nowhere.* There is some very sophisticated analysis of the EBSD data in this paper. I'm sure it took a lot of time to work out and enact. Some of it really does not add anything (I cannot see any impact on the conclusions) and just makes the paper much harder to understand. In particular I see no value in figures 5, 7 and the two central columns of figure 9/A4 and the text that goes with these figs or figure elements. I have

commented on fig 8 earlier. The key scientific points from Figs 9 and A4 are best made by the first and fourth columns alone. Indeed I made a composite of A4 to try and understand better the data myself. I've attached my simplified fig 9 to this review and I suggest a single figure of this form will help you explain the misorientation data and it's significance much more clearly. Similarly I made a compacted version of fig 6 (also attached) to understand better what these data show. The Solid Earth readership is not the place to explore the much more sophisticated analysis I have suggested you cut (see annotated pdf). It will take a lot of work to make these approaches intelligible and further work (and space) to make it clear what scientific value they add. If you can demonstrate the value of these approach I think you should publish them – but in a journal for a more specialist audience.

7. *Describe the "plots" at the point where they are used*. The methods section includes the descriptions of the plotting approaches. When reading the results one has to constantly refer back to the methods. I would use the methods for the experiments and EBSD acquisition and processing (bring out of appendix) and describe the plots where they are presented in results. I think this will make the paper clearer and shorter.
8. *Discussion: needs a figure and shortening.* The discussion attempts to present a model to explain the CPO transitions the authors have documented. The effectiveness of the discussion will be improved by
    a. Having a cartoon figure that reminds the reader of the key observations and the presents the model built open these (much like a graphic abstract).
    b. Shortening (a lot) and tightening. The discussion is way too long. A paper can only make so many key points effectively and this discussion is far too expansive. The effect is the reader will take very little away from the paper. I have drafted what I think are key data points from my reading and suggest that these form the framework of discussion.
9. *Make real conclusions.* The conclusions do not really give the reader any useful idea of what you have found out. They are a mess.
10. *Fold the appendices into the main text.* I don't think you have anything that needs go into an appendix- it is all better in the main text – especially if number of figures reduced.
11. *Simple writing.* The writing style is verbose. Sentences are too long. Complex phrases are used where simple ones would work better. I have highlighted examples on the annotated pdf. Overall the writing lacks clarity and needs considerable improvement.
12. *Literature interpretation versus observations.* The discussion of the literature (particularly in the introduction and discussion) tends to focus on the interpretations of particular papers, sometimes without explicit reference to the data or observation that leads to the interpretation. For completeness and to enable better comparison to your new data literature citation needs to refer to both observations and interpretations.

Here's some key data points I get from the paper. I started writings this as a framework for my own understanding (because I could not extract this easily from reading the paper) and as a potential replacement for your conclusions. What I have here is too expansive for conclusions, although it could be a framework for the discussion. If data (figs etc) do not have a direct line through to conclusions they should be omitted.

Firstly some simple factual conclusions- should not ever be wrong. 2 to 5 could be put as one. A summary figure could schematize these characteristics

A. CPOS and microstructures, from EBSD data, are presented for three experimentally deformed quartzite samples, sheared to similar high strains in regimes 1, 2 and 3.
B. The samples show a transition in CPO. In regime 1 [c] axes are clustered around a direction (B-fibre) rotated a few degrees away from the normal to the shear plane. In regime 3 the [c] axes are clustered in the shear plane and normal to the shear direction (Y-Fibre: parallel to vorticity axis). The CPO of the regime 2 sample is transitional.
C. In all regimes the most significant <a> cluster is in the plane that contains the shear direction and the shear plane normal. The cluster lies at an angle of ~10 degrees from the shear plane, with a rotation sense compatible with vorticity.
D. The {r} rhombs are clustered around an orientation close to the maximum principal stress direction in regimes 1 and 2 and have a much weaker alignment in regime 3.
E. CPO strength increases from regime 1 to regime 3.

Then on to some more sophisticated observations. Still factual. These are more subtle points that I think are quite new and maybe important in interp. Again inclusion in a schematic diagram will help here.

F. In all three regimes CPO strength is higher in grains with higher intragranular deformation intensity as measured using a grain kernel average misorientation (gKAM). In all three regimes the ratio of the number of Y domain to B domain grains increases with intragranular deformation.
G. CPOs have been generated for data subsets with limited ranges of grain size, aspect ratio and long axis orientation. These show that strongest CPOs are developed in populations of grains with the highest aspect ratios and with long axes aligned close to the orientation of maximum elongation. These statements apply to all three regimes.
H. CPO strength increases with increasing grain size in all three regimes although this effect is stronger in regime 1 than regime 3.
I. Low angle misorientations within all grains lie dominantly parallel to the vorticity axis. Misorientations in the crystal reference frame depend on the grain orientation. Misorientation axes in Y domain grains cluster around [c], whilst those in B domain grains lie dominantly in the basal plane, with concentration around {m}. These observations are generally true of all regimes.

J. Something about <a>transparency if a useful point comes from this
K. Something about Schmid factor analysis (see fig with comparison to Little et al data)

Then onto interpretations. I am bit lost here as I'm not really clear what are your key conclusions. The conclusions in the paper certainly do not tell me. Needs to be structured as

L. Interpretations made from your data alone
M. Interpretations that bring in outside information (e.g. strain series information)

I hope this review is useful.

Refs cited in review and listed on annotated pdf.
(Kunz et al., 2009; Little et al., 2016; Pehl and Wenk, 2005; Qi et al., 2017)

Cross, A., Hirth, G., and Prior, D. J., 2017, CPO evolution: effects of secondary phases and grain boundary sliding: Geology, v. doi:10.1130/G38936.1

Heilbronner, R., and Tullis, J., 2006, Evolution of c axis pole figures and grain size during dynamic recrystallization: Results from experimentally sheared quartzite: Journal Of Geophysical Research-Solid Earth, v. 111, no. B10.

Hirth, G., Teyssier, C., and Dunlap, W. J., 2001, An evaluation of quartzite flow laws based on comparisons between experimentally and naturally deformed rocks: International Journal of Earth Sciences, v. 90, no. 1, p. 77-87.

Hirth, G., and Tullis, J., 1992, Dislocation Creep Regimes in Quartz Aggregates: Journal of Structural Geology, v. 14, no. 2, p. 145-159.

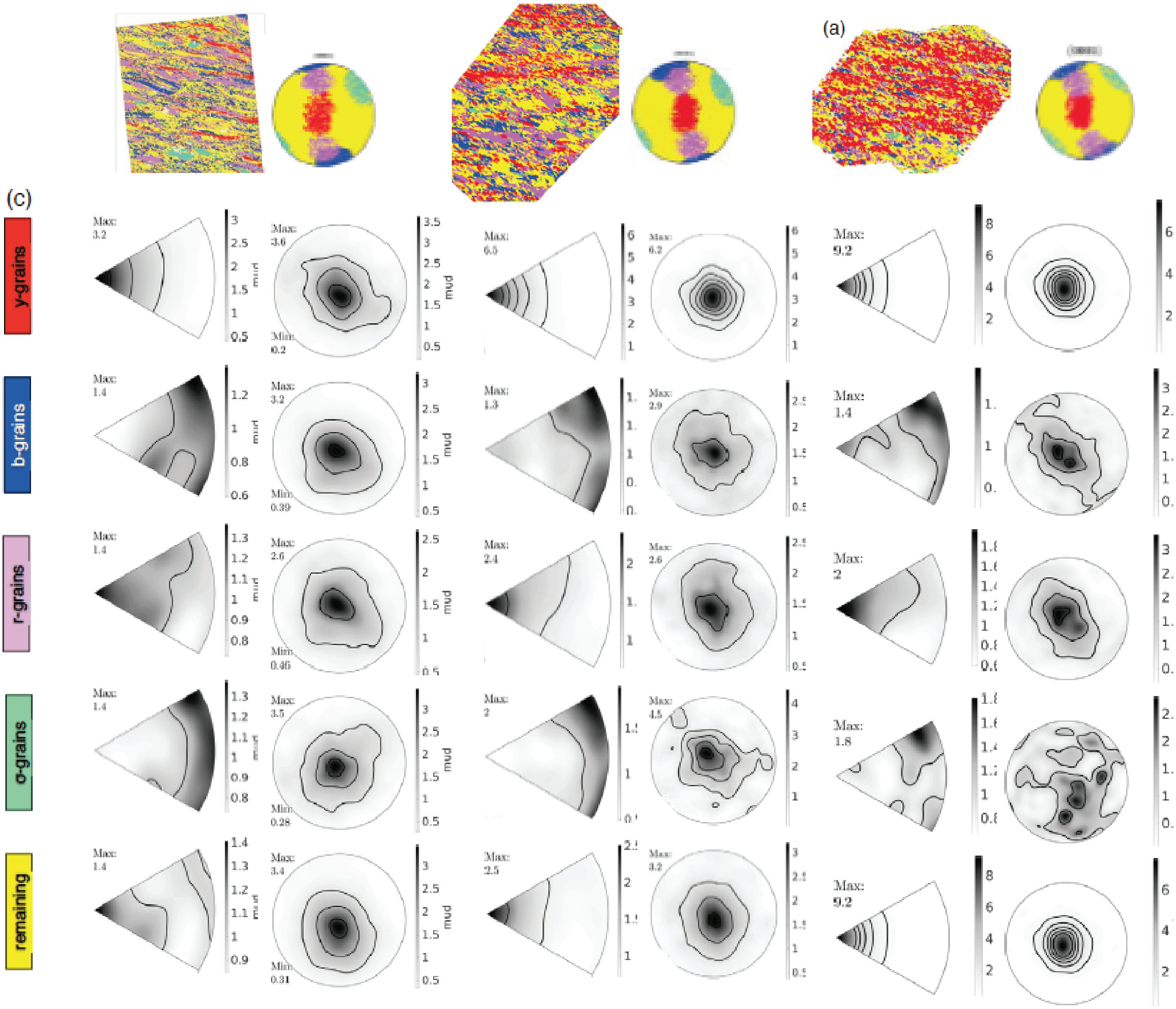
Kunz, M., Chen, K., Tamura, N., and Wenk, H. R., 2009, Evidence for residual elastic strain in deformed natural quartz: American Mineralogist, v. 94, no. 7, p. 1059-1062.

Little, T. A., Prior, D. J., and Toy, V. G., 2016, Are quartz LPOs predictably oriented with respect to the shear zone boundary?: A test from the Alpine Fault mylonites, New Zealand: Geochemistry Geophysics Geosystems, v. 17, no. 3, p. 981-999.

Pehl, J., and Wenk, H. R., 2005, Evidence for regional Dauphine twinning in quartz from the Santa Rosa mylonite zone in Southern California. A neutron diffraction study: Journal of Structural Geology, v. 27, no. 10, p. 1741-1749.

Qi, C., Goldsby, D. L., and Prior, D. J., 2017, The down-stress transition from cluster to cone fabrics in experimentally deformed ice: Earth and Planetary Science Letters, v. 471, p. 136-147.

Trimby, P. W., Prior, D. J., and Wheeler, J., 1998, Grain boundary hierarchy development in a quartz mylonite: Journal of Structural Geology, v. 20, no. 7, p. 917-935.

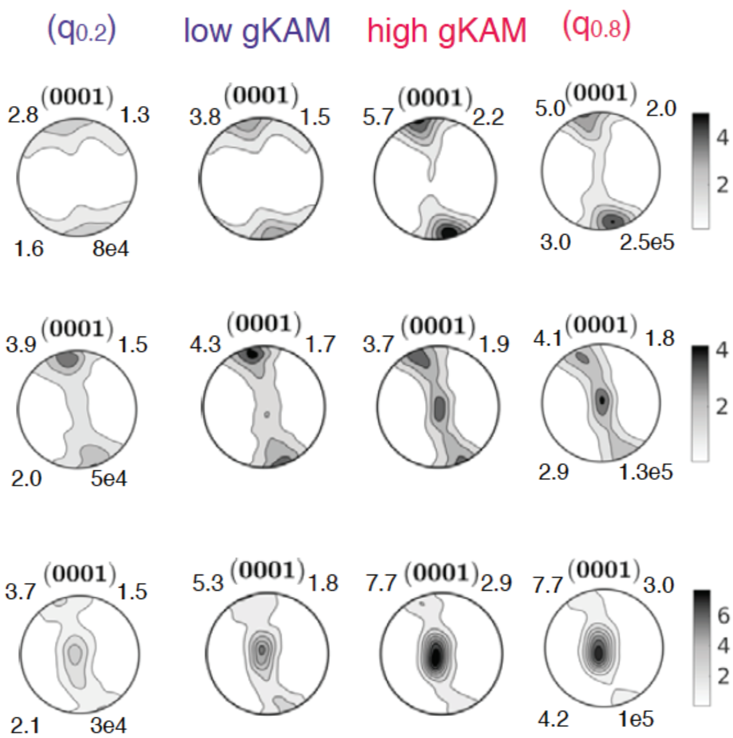


if all contoured with same intervals fewer legends needed. Also the grey scale variation does not show the casual reader that the y grain misorientations are all much stronger. Also do each of these data sets contain a comparable number of grains? Or comparable number of point pairs. Caption says drawn from randomly drawn subsets. This does not define what you have done clearly.

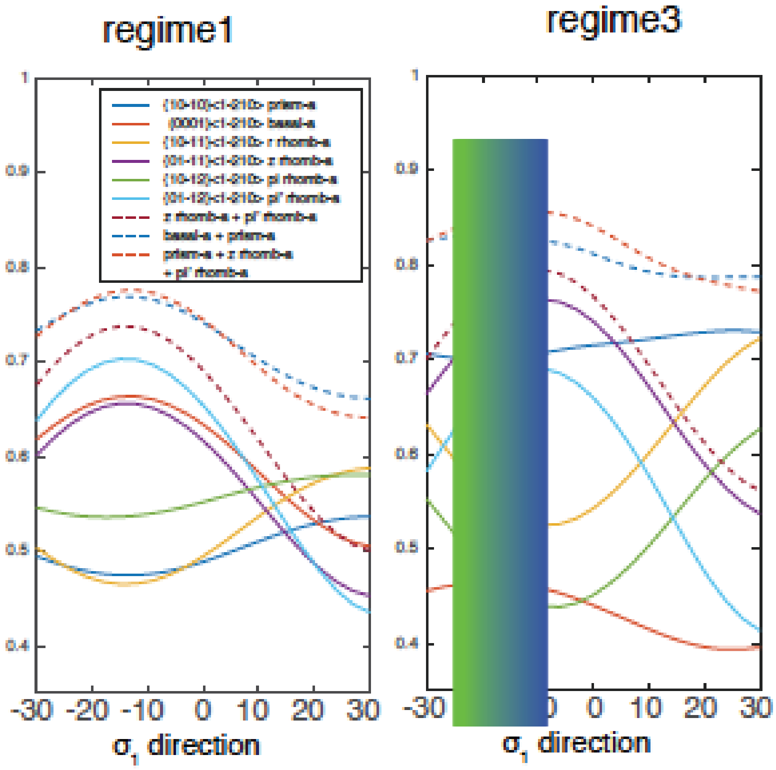
I would include the number of grains in each figure pair

Fromthe PFs in fig 1 I do not expect many grains in the sigma orientation and wonder whether the less organised patterns in reg 2 and 3 relate to this. Similarly

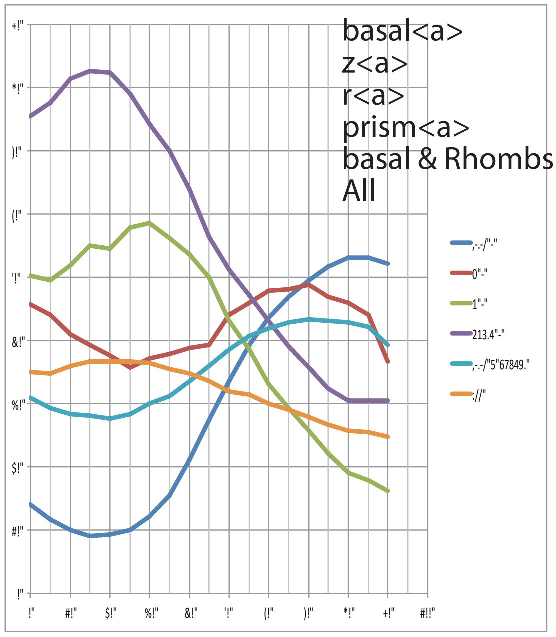
I predict the number of b-grrains to reduce from regime 1 to 3 (from PFs) and wonder whether some of the shape changes here reflect that?

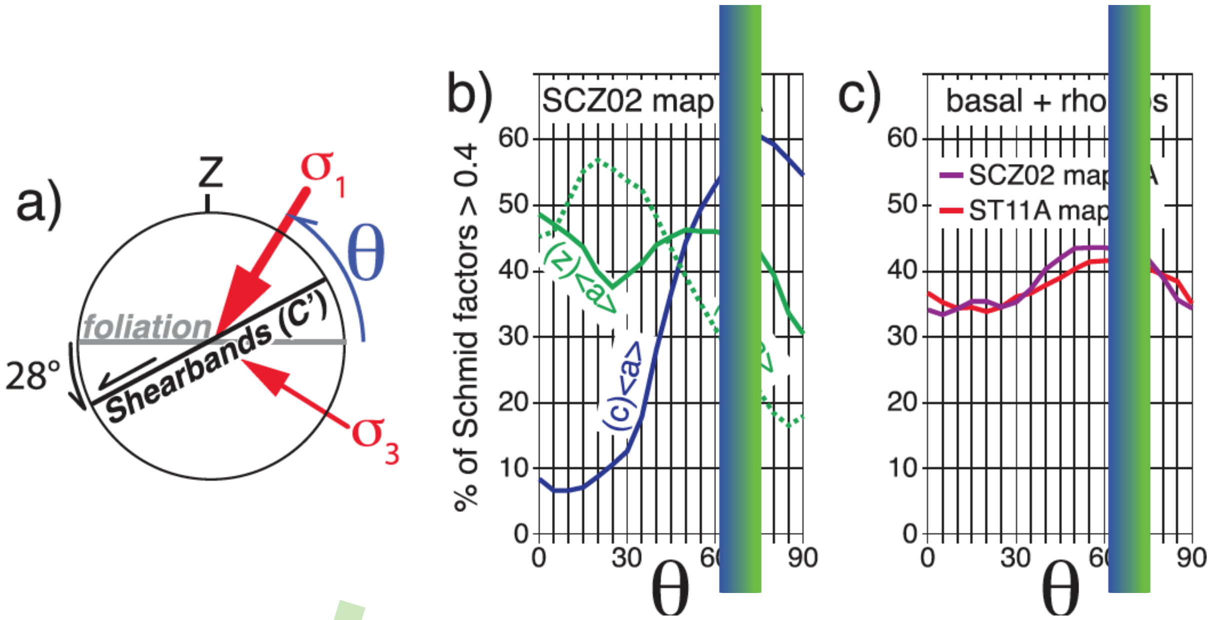


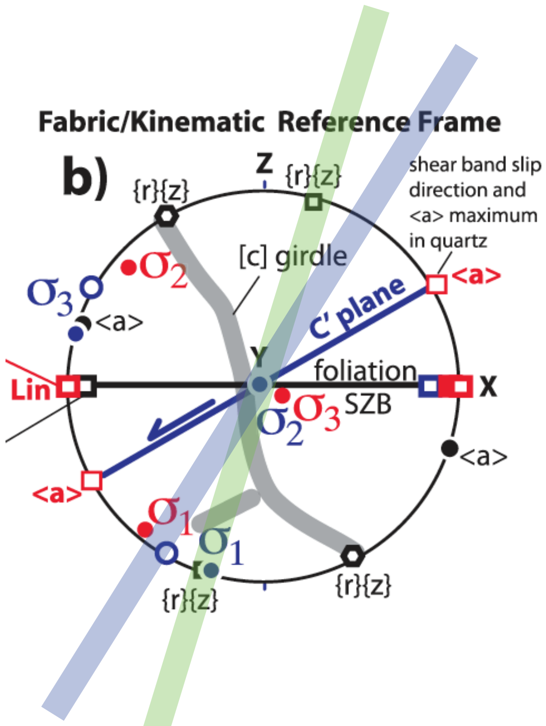
Essential elements of Fig 6 needed. Does not need other directions. I don't think the microstructure pic needed but could be. This gets over the transition from B to Y with increasing intragranular strain.



More than we published: from my data repository. Sorry labels did not translate







COMPARISONS WITH
LITTLE ET AL 2016. I think i've
got the ref frames right to put comparative
purple to green lines on- but I doid this fast!!!