

"Synchrotron FTIR imaging of OH in quartz mylonites" by Kronenberg et al.

Review by Jed Mosenfelder

This is an exhaustive, painstaking study that represents a very useful contribution for people trying to correlate OH contents of quartz to deformation textures. The contoured maps look great and I found much of the discussion about deformation mechanisms and mechanisms for fluid infiltration in section 5 intriguing.

Now for the slightly negative take, I hate to see all of this good stuff buried in a paper that, in my opinion is very long and can surely be shortened by removing redundancy. For instance, nearly 1/3 of the introduction should just be removed, because it is a summary of the results and really doesn't belong in the introduction (it's unnecessary foreshadowing!). On the other hand, much of the methods section should be concatenated with the introduction, because it is not a technical description so much as a justification for why using synchrotron FTIR is useful, which is the whole point of the paper. I know that a lot of my comments are nitpicky and some are almost as wordy as the paper itself, but I hope these suggestions will be constructive for improving the presentation of the paper.

Comments:

1. Line 136: put IR in parentheses here. Same on line 147: put FTIR in parentheses. Then, you can shorten the manuscript non-trivially by using the acronym "FTIR" without saying "spectroscopy" every time, which is redundant and kinda grating. Speaking of grating, practically no one these days uses a grating spectrometer for IR so I think it is ok to say "FTIR" when you are being general, e.g. you can use just "FTIR" instead of "IR spectroscopy" in line 172.
2. Line 179-196: I feel quite strongly that this verbiage can be eliminated, as alluded to above. It's a summary of your results, which is not needed in an introduction. In fact, reading something like that just makes me want to skip reading the rest of the paper!
3. Section 2: the geologic background section is also very long. I guess your readership laps this stuff up though so if you feel it is really necessary to review all of these previously studied details of the two field areas, then ok. One thing I wonder is whether you could get away with using "MT" and "MCT" as acronyms throughout the paper to reduce the character count and eye fatigue associated with repeating Moine Thrust and Main Central Thrust so much.
4. Line 207: better fill in citations for OTHERS? here
5. Line 292-327: On the one hand, much of this was already said in the introduction and should not be repeated here (e.g. the long list of references citing people who used FTIR in the past). On the other hand, some of the schpiel here could be moved to the introduction as I say above in my summary.
6. Line 329ff: WOW this is the longest sample preparation I have EVER read! While much of this could be interesting to technical wonks such as myself, at the risk of repeating myself ad nauseam I think some of it could be reduced. To me,

- the most interesting steps involve your methods for mechanically supporting the samples, not the entire sequence of grit sizes you used. You can also say in maybe just one or two sentences that you checked thicknesses using optical methods.
7. Line 404-411: I don't think this detail is necessary. I hope people who use these machines already understand that they can collect data out to 7400 cm^{-1} (actually I wonder sometimes if they do), but who cares? It is totally irrelevant to your study, you just need to say what range you collected (saved), and the resolution and number of scans (512 or more I guess). And you also don't need to say you normalized the spectra, that detail can go in figure captions.
 8. line 435: I am feeling un-experty here but I am not sure I have ever seen an IR source being described as "isotropic" or "anisotropic". The light that comes into your sample is not polarized and frankly I am not sure what you are getting at here. Incidentally, Rossman doesn't like using the word "pleochroic" (I guess "dichroic" is indeed appropriate for uniaxial quartz) in this context as it implies the presence of color ("chroic"), which we do not see in the infrared part of the spectrum. But I am not so nitpicky myself, believe it or not, even though I have stopped using it in my own papers.
 9. Line 484ff: the odd thing about this section (which I know is important to the paper) is that the spectra you refer to in figure 2c really don't have such bad fringes! In later figures you show more extreme examples. I wonder if you want to reorganize the figures, discussion, and/or figure call outs to make your point more strongly.
 10. Line 535: strictly speaking you are not accurately separating the absorbance of mica from fluid inclusions in quartz. No way. That's because the bands overlap (they are broad bands with full width half maximum positions that overlap), so if you just draw a line like you did in figure 3a then you are underestimating the integrated absorbance of the mica. The proper way to do it is to actually fit the bands with gaussians and/or lorentzians, etc. I can't believe it matters to your conclusions and I can't believe you would want to go through the heartache of properly fitting the bands, but I also don't think you should claim that you are ACCURATELY subtracting the absorbance of the mica. This is the kind of thing I did in my dissertation 20 years ago when I was extremely naive.
 11. line 546: maybe I am blind but I am not seeing a band at 3815 cm^{-1} and would be curious to know what it is, it seems like a very high frequency for O-H.
 12. line 571: I don't think you need to cite TWO textbooks for something so well established as the Beer Lambert law (I would have neglected to cite any here)
 13. Line 604: this entire discussion is a little goofy, because inherently you also do not know the path length for the inclusions so of course there is no way to quantify the amount of mica present. I suggest trimming this paragraph down.
 14. line 665ff: I wonder if you want to shout out to your figures here where the contouring with cool and warm colors is shown. It might put your figures out of order but it makes sense to me anyway to draw the reader's attention here to your pretty pictures.
 15. Line 700ff: It is kind of "no wonder" that you see the same bands when using synchrotron IR as opposed to a bench top FTIR, so I think you could reduce a lot

of this verbiage. I mean, were you seriously expecting to see different O-H vibrations? Of course not.

16. line 754: the method of tilting the plate by 45 degrees is curious to me. I assume you compensate for the change in path length by doing simple trigonometry here but maybe you want to actually state that for clueless readers like me? I can't believe I am actually asking you to add something to this paper ;-)
17. Line 768ff: this seems to be an interesting by-product of your study that could be quite useful to people in this field and so I wonder whether you want to draw attention to it with a sentence or two in the abstract.
18. line 810: imaging, not imagining, unless you are Disney. No shoot, that's imagineering ;-)
19. Line 950: Seaman spelled wrong here
20. Line 999: copy editing trivia here but I am not sure why Holger's paper is underlined
21. line 1030: well, this is an interesting idea but it is a purely hypothetical concept and I cannot think of any practical way to do this so I am not sure it should be in here. What is the material you are thinking of that has the same index as quartz and yet is IR transparent AND can somehow magically bond to the sample (by melting? seriously? Not gonna happen for CaF₂ or BaF₂ etc. There is no material I can think of with a low melting temperature, such as a plastic, that will also have a high refractive index) so there is no air gap, without risking affecting the OH content? Nutty.
22. line 1042: I like this visionary idea better but it sure is going to get expensive with all those sections you want to look at ;-)
23. section 5.1, 5.2, and 5.3: the geological implications for sections 5.1 and 5.3 are important and the technical discussion in 5.2 sort of sits uncomfortably between them. I would consider just moving the sections around so that 5.1 and 5.3 are together (maybe at the end rather than the beginning? I dunnow).
24. figure captions, general comment: wow, they are way too long (particularly figure 3). Much of this information repeats what is said in the text. My general philosophy about figure captions is that you should try not to repeat too much of what is said in the text and try not to have too much interpretation within the figure caption - the goal is to just describe the facts of what you are presenting (for instance noting that spectra are normalized and offset is ok - in fact you can just say "spectra normalized to 1 mm thickness"). I got this philosophy from working with Tom Ahrens who totally hammered on me about this and I came to totally agree with him about it.
25. figure 3b: I may fundamentally misunderstand this. Is this spectrum the result of subtracting away the OH in quartz or is it actually a spectrum of pure mica? If the former, then it just demonstrates how my complaint about your subtraction is valid, because the right side of the band looks abruptly cut, in other words there should be a tail of absorption on the low wavenumber side but it abruptly dives to zero. I think this is an artifact of your subtraction method but I am not sure.
26. Figure captions for figures 6-8: I think a lot of the detail is repeated (such as the scale for the contours, the units for OH, the "cool" versus "warm" coloring, etc) and can be said just in the first figure caption, which is referred back to.