GEOCHRONOLOGY
Discussions

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Interactive comment on "Resolving the effects of 2D versus 3D grain measurements on (U-Th)/ He age data and reproducibility" *by* Emily H. G. Cooperdock et al.

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Response to: Interactive comment on "Resolving the effects of 2D versus 3D grain measurements on (U-Th)/ He age data and reproducibility" by Emily H. G. Cooperdock et al. Christoph Glotzbach (Referee) Âǎchristoph.glotzbach@uni-tuebingen.de Received and published: 14 June 2019

Please find our responses below each comment. We also attached a revised version of the manuscript and additional appendices with tracked changes to this review.

General comments Dear Authors, Overall I found the manuscript well written, struc-

tured and the topic is of interest for the thermochronological community. The applied analysis is of high quality, but lacks some comments on accuracy and general applications to 'normal' samples (fewer grains). See my Scientific and Technical comments below for details.

Scientific comments

1) I am not totally convinced that the 3D-CT measurements are accurate enough to judge the quality of 2D measurements. The resolution of the voxel is 4-5 m, relatively large compared to a typical grain size of 100 m. The authors should convince the reader that the resolution is high enough to use their CT measurments as reference. Maybe you provide some real/synthetic data to prove that the resolution is good enough. You have provided some information in the text, but I am not totally satisfied with that.

Response: We have added a detailed summary of tests that address these concerns as Appendices B and C, and with Figure B1. In sum, we show that our implementation of measuring grain radii and FT in Blob3D provides a high degree of accuracy and precision even on very small grains at low resolutions where voxels are 20% of the grain radius.

2) You have estimated the hexagonal cross-section assuming an equal-sided hexagonal cross section and state correctly that this is not an adequate assumption for all grains. Since it is quite easy to measure the cross section for each grain with a bit more effort, please state why you haven't done this and/or calculate for extreme cases how much uncertainty you add by assuming the equal-sided cross section.

Response: Point well taken – Although some labs do measure the third dimension, we note that many labs do not routinely do so. As measuring practices vary by lab, we chose to mimic the simplest measuring technique for comparison with the 3D CT data.

3) You conclude that although estimates of volume, surface area, ESR and Ft are

deviating significantly for individual grains they partly average out or in average (for all measured grains) do not deviate from the CT derived values. You have not considered that the usual amount of grains measured in a bedrock sample is around 3 or 4 and in this case the deviations you observed are very likely not cancelling out. You could for instance provide the reader with some estimates of the possible deviation for 3-4 grains by (1) randomly resample 3-4 grains for each sample and (2) calculate the deviation from the complete dataset of different parameters (e.g. ESR, Ft). I hope you find my comments and suggestions helpful.

Response: We have addressed this suggestion by taking the average of four random grains from each sample 1000 times for Mean Ft and Age. The results of this are added to Figure 7, Table 2, and discussed in the text in sections 4.1.4 and 4.2.

Technical corrections: Page 2, Line 10-30: No references here, please add relevant references.

Response: References have been added.

Page 3, Line 3: Herman et al. (2007) and Glotzbach et al. (2019) did this before.

Response: Herman and Glotzbach are cited on this sentence now.

Page 3, Line 5: You do report results from the study of Evans on the accuracy of Ft values, why not reporting results from Glotzbach et al. (2009) on grain measurements?

Response: A sentence is added that reports the Glotzbach results on Ft.

Page 7, Line 6: Not all reader might know what you mean with UFt and ThFt, please explain and probably use U-Ft and Th-Ft which is easier to read.

Response: UFt and ThFt is referenced to Farley et al., 1996, which has an explanation of the derivations of the equations. We tell the reader to reference this in section 2.4.1.

Page 7, Line 7: Some or most of your grains do have tips, why have you not included them in this calculation? There are equations to do that, e.g. Ketcham et al. (2011).

Response: We purposefully chose to compare the 'simplest' 2D measurement approach with the 3D data, with the idea that it will provide an important point of comparison as many labs use this approach.

Page 7, Line 8: Here you use W for half-width, but further in the equations you use r. Please be consistent.

Response: This has been changed to "r".

Page 7, Line 18: I would prefer to write ESR = 3 * V/SA

Response: This is changed.

Page 7, Line 21: My understanding is that the density of apatite is closer to 3.2 g/cm3, maybe 3.18. A reference would be nice to have.

Response: This is a typo and now has been fixed to 3.2.

Page 7, Line 23: Give reference, e.g. Farley 2002.

Response: This has been added.

Page 8, Line 10: Please can you add a few examples of how you fit the CT-scanned grains with boxes. Please show examples where this method works fine and if present also some examples that could maybe not fit that easily.

Response: We have added as Appendix C a discussion and animation that demonstrates the way Blob3D fits boxes.

Page 9, Line 18: Do you start from the center of the voxel, or somewhere within the randomly chosen voxel? Since the voxel resolution is not that high (4.6-5 microns), starting from the center of the vexel may bias the calculation. Please clarify.

Response: We've clarified the text to state that we first randomize which voxel, and then randomize the location within that voxel.

Page 9, Line 25: If stopping distance/voxel size > 4 means the resolution is high, the

sign should be opposite <!? Can you clarify for which sample/isotope this is true for your dataset and when you have used this supersampling approach.

Response: Sign switched. We've also clarified that we use the 238U stopping distance for this test. Appendix B describes super-sampling in more detail.

Page 10, Line 32: Although the result will be quite identical, you have to correct the He content and not the uncorrected age (put the ejected He back in the grain).

Response: We have noted this comment, but decided to leave the text as-is, e.g., Farley et al., 1996.

Page 11, Line 15-18: I would simply omit the grain and you can delete this section.

Response: We chose to leave this grain as part of the discussion of the introduction of user-error. We added some text to say how the importance of user error will vary by lab, microscope, software, etc.

Page 11, Line 29-30 and Page 12, Line 1: How serious is this issue, please report how this can happen and how often and to what degree. You could make repeated measurements on the same grain. Our microscope system is saving the magnification of each picture taken and we do not have yet found any errors. Please also have a look if the grains are somewhat different from other grains (more complex geometry).

Response: This issue is going to vary widely in different labs due to the variety of microscopes and software used. In this case, it was an older software that did not record the magnification. Text has been added to qualify that the issue of 'user error' will vary widely by lab. We bring it up because it ended up being an important source of error in our study, and an issue that needs to be addressed lab-by-lab.

Page 15, Line 6: Please explain what you mean with simple geological histories

Response: The geologic histories are explained in the Background section. By this we mean that they come from crystalline samples that experiences relatively fast exhuma-

tion and no subsequent known reheating. This sentence has been revised.

Page 15, Line 18: Please explain why you have not used the equations of Ketcham et al. (2011) and did some measurements of the hexagonal cross section, e.g. using double-sided tape. On page 16, Line 20 you indirectly suggest that this should be done.

Response: We recognize that different labs have different protocols for grain measurements on the microscope. We chose to measure the grains this way because it is commonly practiced and has the greatest amount of assumption built into it, thereby we expect to see the largest possible deviations

Page 17, Line 10-12: This might be true for the average, but we should still care about the deviation of single grains since deviations might not cancel out if only a few grains are analyses. I would suggest you to randomly (maybe 1000 times) sample 3 or 4 grains from one sample and measure the mean deviation in Ft for those grains. Make a figure with deviation in Ft (x-axis) against probability (y-axis). In this way the results can be better transferred to normal bedrock samples.

Response: We have added this analysis of the data to Figure 7 and discussed it in the text in sections 4.1.4 and 4.2. In short, our 1000-test trial showed that the overall population results with 1-sigma uncertainty we reported match that of the 4-grain trial runs well.

Page 18, Line 7: Where do you get this from, please provide some evidence for this conclusion (refer to a figure or table).

Response: We have added Table and Figure references to this section.

Page 19, Line 7-9: Make sure you pronounce that this is really only true for these two samples (with fast cooling history). I would expect that even though inclusions may not be always of minerals with high U-Th concentrations they still have a considerable effect on He diffusion. Please mention this to make sure that the reader does not get it wrong and start to pick grains with inclusions.

Response: We've changed the sentence to make it more direct that inclusions can be (and often are) a source for dispersion, just not in these samples apparently.

Page 19, Line 14: Please provide the reader with some figure that supports your conclusion. To help the reader to better estimate the importance of broken grains, please report how large the deviation in Ft will be for a range of broken grain scenarios. Maybe you calculate for a few grains of your samples the Ft assuming that the grain broke (1) during mineral separation and (2) broke before cooling. We presented a method to account for this (e.g. Fig. 9 in Glotzbach et al. 2019) and show an example that yield a deviation of 'only' 5% which might be not detectable with your dataset since it is in the same range as other uncertainties.

Response: We do not include a plot of the grain habits vs age because we thought it wasn't more informative than the information provided in Table 2. This study was not designed to assess the effects of broken grains, as few grains within our samples exhibited clear 'broken' ends. This is also supported by the relatively high reproducibility of aliquot ages, and we do not note any specific trend with 'older' ages and broken-looking surfaces. In any event, our software is not yet in a state where it can attempt to "complete" broken grains, which is a difficult problem when habits vary greatly. As such, we do not assess the effect of broken grains and Ft corrections in detail.

Page 19, Line 29-31: I am not an expert, but I guess you also have to calibrate a CT-scanner or?

Response: Modern CT scanners should not need to be calibrated, but we have added a paragraph that discusses user inputs and best practices and pitfalls.

Page 20, Line 11: The optical microscope along cannot measure eU, please add that you have used an ICP-MS.

Response: Yes, eU has been removed from that sentence.

Table 1: Can you also report the difference (with sign) not only the absolute of it. Not

sure if you really have to report the U Ft and Th Ft, just show the total Ft.

Response: The positive or negative difference is shown in the 3D/2D fractions, where 3D/2D < 1 is equivalent to a negative difference, and 3D/2D > 1 is related to a positive difference. Then the absolute percent is reported to highlight the magnitude of difference.

Fig. 5: Could you colour-code the relative differences (deviation from the 3D model) and make a small legend in one of the plots?

Response: We revised Figure 5 by adding contour lines to the graphs that shows the % difference.

Please also note the supplement to this comment:
https://www.geochronology-discuss.net/gchron-2019-3/gchron-2019-3-AC1-supplement.pdf

Interactive comment on Geochronology Discuss., https://doi.org/10.5194/gchron-2019-3, 2019.