Response to RC1 Comments

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Jan. 20, 2025

I thank the reviewer for their comments and feedback on the manuscript. Most of the comments deal with clarifying and providing more explanation of the overall approach and using more explicit, less ambiguous terms. I see no problem implementing these changes and believe they will greatly improve the manuscript. I think it likely that many readers of the original manuscript will have similar questions and comments as RC1 and am providing responses here to help clarify prior to the end of open discussion. I will provide additional responses after incorporating other feedback.

RC1: From what I understand from your manuscript, your proposed approach will likely under- or overestimate the Ft value since you are using volume and surface area calculation of the polished grains for your calculation of Ft. The correct Ft value is dependent on both the original grain geometry and the resulting after polishing and only if half a grain is polished both will be similar. The resulting Ft value calculated with your approach will be smaller than the corresponding Ft value of the whole grain, in case polishing removes less than half of the grain. The opposite is in case more than half the grain is removed during polishing. Either show the difference to the correct value and state the limitation or implement the correct calculation.

AC: My approach is intended to provide an F_T correction for the grain fragment remaining after polishing rather than the whole original grain, regardless of how much of the grain remains. Since only the fragment is analyzed for conventional bulk U, Th, Sm, and He measurements, applying an F_T correction based on the original, unpolished grain volume and surface area would be inappropriate without also somehow correcting these isotopic measurements to reflect the original whole grain morphology. Although this is theoretically mathematically feasible, the uncertainty associated with doing this – both quantifiable and unquantifiable – make it a worse option in my opinion than proceeding with just the direct measurements of the remaining fragment as done here.

I can see that this basis of the approach presented – calculating values for the polished grain fragments, not the original whole grains – was not communicated effectively in the original manuscript and I will emphasize this explicitly in revisions.

RC1: Line 1,16: Specify what you mean with ‘derived value calculation’. Also, later you often say something like ‘other values’. Please make sure that you always specify the measurements you are referring to.

AC: Thank you for pointing out that “derived value” is vague and should be avoided or better defined. Here, I am using “derived values” in a manner similar to Flowers et al., (2022) to refer to data or correction values such as F_T that are not directly measured but are derived from direct

measurements, typically during “data reduction” steps of (U-Th)/He thermochronology workflows. Where appropriate, I will reference just the specific values being discussed. It is still sometimes necessary to refer to this category of values derived from direct measurements as a whole, but I will add a sentence explicitly defining this categorization.

RC1: Line 8-17: You state that the proposed protocol is beneficial for in situ measurements (line 14) and later for bulk grain (e.g. line 16). Please state clearly which method (in-situ and/or bulk grain) would benefit.

AC: The protocol is beneficial for bulk grain conventional (U-Th)/He thermochronology applications in which additional in-situ measurements on the same grains are also required/desired. Examples of complimentary in-situ data collection can include LA-ICPMS or SIMS U-Pb dating or trace element analysis, cathodoluminescence or backscatter electron imagery, etc. I will reword sentences in the abstract and introduction to clarify cases in which the protocol presented is helpful.

RC1: Line 49-50: You may want to reference to my approach using a set of orthogonal microscopic pictures to derive whole-grain geometries (Glotzbach et al. 2019 – Chemical Geology).

AC: Thank you for the suggestion; apologies for the oversight.

RC1: Line 48-58: Please clearly state what your approach is. Measuring only after mounting/polishing or, what I guess, two measurements are required before and after mounting/polishing.

AC: The approach uses one set of measurements made after the grains are polished. This will be explained explicitly in the Introduction and Section 2. Measuring once after grains are polished adds minimally to sample preparation time and avoids introducing additional opportunities for grain selection bias, which can be especially problematic in some applications such as detrital zircon provenance analysis.

RC1: Line 72: The word ‘irrelevant’ is somewhat misleading here, since the depth to which grains are polished is impacted V, SA and other related parameters and is not irrelevant. I guess you mean that it is easy to account/correct for.

AC: I agree better wording is needed here. In some cases, polishing depth is not needed since the volume and surface area of the remaining fragment can be easily calculated from measurements of the fragment alone. In other cases this is not possible and polishing depth is needed.

RC1: Line 74-77: See above, in case you measure individual grains before and after mounting/polishing this would not be required. Therefore I guess you are measuring only after mounting/polishing and derive the depth of polishing from the glass beads.

AC: Yes, grains are only measured after polishing. The Abstract, Introduction, and Section 2 will be revised to state this explicitly.

RC1: Line 85-90: I do not fully understand how you can estimate the correct values of a and b for an ellipsoid (r for cylinder) in case more than half of the grain is polished away. The equations that you state will be minimum values for a and b (e.g. b=W1/2).

AC: Thank you for this feedback, which illuminates that a key point about how the method is applied has not been communicated effectively in the original manuscript. The classification of grains as either ellipsoid, tetragon, or cylindrical geometries relates to the original geometry of the whole grain, prior to polishing. However, the calculation of volume and surface area relates just to the grain fragment remaining after polishing. Volume and surface area calculations are related to the original grain geometry in the sense that the geometry of the polished fragment reflects this original geometry, but do not necessarily use values a, b, c, (ellipsoids and tetragons) or r and h (cylinders) related to a, b, c, r, or h, of the original geometry – these values are defined for the fragment. This clarification will be added to Section 2 and elsewhere as needed.

To address the specific points raised in the comment:

In the case of an originally ellipsoid grain polished more than half away, the geometry of the remaining fragment is approximated as half an ellipsoid with semi-axes a and b determined using measurements of the *remaining fragment*. The semi-axes of the original whole grain and polishing depth are not used. I agree language clarifying that this is an approximation should be added.

In the case of grains that are originally cylinders polished parallel to the c-axis, I also agree that the approximation for r and subsequent volume and surface area derivations presented in the original manuscript are not the best approximations possible. An explanation of a better approach that does not attempt to tie volume and surface area of these grain fragments to equations for a cylinder but instead treats them more simply as prisms with half-ellipse cross sections is included at the end of this reply. This updated approach for cylindrical grains will replace the existing approach in the revised manuscript and R script.

RC1: Line 86: Specify what the ellipsoid coefficient is.

AC: The ellipsoid coefficient is a feature of Knud Thomsen's formula to approximate ellipsoid surface area employed in Ketcham et al., (2011) and adapted here. I will add a fuller citation of this value in the revised manuscript.

RC1: Line 114-115: Same as for the ellipsoid does apply for a cylinder, it is not possible to correctly determine r when more than half the grain is gone. The equation that you are using r= min(W1,W2) will underestimate r. Why not using equation 1 to estimate the correct radius?

AC: I agree this approach is not optimal. A better approach is described at the end of these replies as in the previous response to the Line 85-90 comment.

RC1: Line 158-186: It is unclear to me if you calculate the Ft for the whole grain or the mounted/polished grain. The Ft value of mounted/polished grains will in most cases be

higher/lower than the theoretical value of the whole grain (similar only if exactly half the grain is removed).

AC: F_T is calculated for the polished grain fragment only. The manuscript will be revised to explicitly state this.

RC1: Line 187: Please add more details on how you did the comparison, are this read data or synthetic data and give details how the methods of Ketcham and Reiners differ from your approach.

AC: Thank you for the feedback that more details are needed. The data used is real dataset acquired for a detrital zircon sample. I agree real vs. synthetic data is an important distinction that should be explicit. The Ketcham method is already described in Section 2 in contrast to my approach. I will clarify Section 2 to more clearly differentiate between them and reference that description in Section 5. Adding details about the Reiners method is not a problem.

RC1: Line 189: Please clarify what you mean with 'uncorrected method'?

AC: Thank you for the feedback that this is unclear. The use of "uncorrected method' in this context was meant to differentiate the method of Ketcham et al. (2011) for calculating volume, surface area, and F_T for whole grains from my protocol for calculating these values for polished grain fragments. As stated throughout the text, my protocol draws heavily on the approach and equations employed by Ketcham et al. but modifies them so that they are correct for polished fragments. However, based on this and other comments, this wording has only created confusion. The revised manuscript will refer simply to the "Ketcham et al. method" in contrast to the method presented in the manuscript.

Updated volume and surface area for cylindrical grains polished parallel to c-axis

For grains that are originally cylindrical and polished parallel to the c-axis, the removed portion of the grain or grain fragment remaining, depending on degree of polishing, can be approximated as prisms with cross sections perpendicular to the c-axis that are half ellipses (see diagrams in Table 1 below). Using this approximation, the volume and surface area of the remaining polished grain fragments are calculated using the area of an ellipse ($A_{ellipse}$, Eq 1) and Ramanujan's Formula for the approximate perimeter of an ellipse ($P_{ellipse}$, Eq 2). Updated equations for the volume (V) and surface area (SA) of originally cylindrical grains incorporating Eq 1 and 2 are given as Eq 4 – 7 in Table 1 below.

$$A_{ellipse} = \pi ab \quad (1)$$

$$P_{ellipse} = \pi(a+b)\left[1 + \frac{3k}{10+\sqrt{4-3h}}\right] \quad (2)$$

Where a and b are the ellipse semi-axes and k is defined as $k = \frac{(a-b)^2}{(a+b)^2}$.

To determine the degree of polishing using the polishing depth g (calculated as described in the manuscript using measurements of polished glass beads), the original radius of the cylindrical grain before polishing is calculated using Equation 3.

$$r = \frac{g + W_2}{2} \quad (3)$$

Table 1 Originally cylindrical grains polished parallel to c-axis volume and surface area calculation. Gray segments in cross sectional diagrams represent grain fragment remaining after polishing for which volume and F_T surface area are calculated.

Degree of Polishing	Cross Section Perpendicular to c-axis	Values Defined Using 2D Grain Measurements	Volume and Surface Area Equations
$g < r$ Polished < halfway		$a = g$ $b = \sqrt{r^2 - (r-g)^2}$ $h = \frac{L_1 + L_2}{2}$ $k = \frac{(a-b)^2}{(a+b)^2}$	$V = \left(\pi r^2 - \frac{\pi}{2}ab\right)h$ (4) $SA = 2\left(\pi r^2 - \frac{\pi}{2}ab\right) + \left[2\pi - \frac{\pi(a+b)}{2}\left[1 + \frac{3k}{10 + \sqrt{4-3k}}\right]\right]h$ (5)
$g > r$ Polished > halfway		$a = W_2$ $b = \frac{W_1}{2}$ $h = \frac{L_1 + L_2}{2}$ $k = \frac{(a-b)^2}{(a+b)^2}$	$V = \frac{\pi}{2}abh$ (6) $SA = \pi ab + \frac{\pi(a+b)}{2}\left[1 + \frac{3k}{10 + \sqrt{4-3k}}\right]h$ (7)