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Reply on RC1

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Author comment on "A revised alpha-ejection correction calculation for (U–Th)☐/☐He thermochronology dates of broken apatite crystals" by John J. Y. He and Peter W. Reiners, Geochronology Discuss., https://doi.org/10.5194/gchron-2022-11-AC2, 2022

Thank you Dr. Ketcham for your thorough review. Our response to the comments and line-by-line suggestions are included below.

“One abiding issue that the authors could discuss more are the ramifications of not knowing when the fracture took place – was the grain broken during the mineral separation process, or was already a fragment in the rock. A further complication to the latter case is whether it was an isolated fragment in the rock, or a part of a larger, fractured crystal, where ejection would be matched by implantation across the fracture interface, but the fracture would also serve as a grain boundary for diffusive loss. How does uncertainty on this point affect the correction? One idea might be to run cases similar to Fig 2 and 5, such as one where “broken grains” were broken pre-deposition and thus should ideally not be corrected; the new protocol increases the overcorrection, resulting in a less salutary histogram of deviations. Accordingly, it would also be beneficial to also discuss, what are the textural clues for discerning when the fracture took place, and how reliable they are likely to be? There are some easy ones, like rounding suggesting transport, but perhaps the authors have additional experience to convey.”

As Dr. Ketcham’s comment suggests, it is not possible to definitively assess when the fracture took place, and this is a fundamental problem for both the new and old protocols. Whether or not to apply a fragmentation correction is a question that precedes what protocol to apply. Nevertheless we agree that this is a significant issue that warrants additional discussion in the manuscript, and will make the appropriate revisions, as discussed below.

For igneous samples, any crystals with existing fractures prior to cooling would most likely still be intact, from an alpha-ejection perspective (i.e. the fragments are immediately adjacent, so long alpha-stopping distances implant He across fractures). This means that the fragmentation correction to a grain that has lost one or two termination(s) would still need to be applied. On the other hand, the question of when the fracture occurred matters for He diffusion. Depending on the thermal history, and whether the fracture pathway was a free surface for He loss, the He concentration profile of the fragment would be the result of some combination of alpha ejection having acted on external non-fragmented surfaces and diffusion having acted on all free surfaces. An additional complication, for certain thermal histories (e.g. partially reset samples), is that a broken face that is still adjacent to the other broken side so that it has not experienced alpha-ejection helium loss, may experience more diffusion at this fracture plane than the exposed external faces where diffusion is inhibited by the lower He concentration at the crystal boundary. We will revise the text to discuss this complication, but it would be beyond the scope of the manuscript to quantitatively model the effect of diffusion along uncharacterized fracture pathways whose diffusive properties are unknown.

For detrital samples the situation is more complicated. For samples such as modern river sands derived from crystalline rocks, in our experience an assumption that c-axis-perpendicular breakage occurred after cooling (through approximately-closure-temperature temperatures) can be reasonably based on textural clues, particularly the contrast between detrital apatite grains that are rounded or abraded by transport and the sharp faces and corners of fragment surfaces that have not. For sedimentary samples that have not been clearly buried and reset, e.g. sedimentary rocks not buried more than couple km, the timing of fragmentation would be more ambiguous, unless the age of the deposition is known (assuming that the age of the deposition is close to the age of erosion and transport, and therefore the timing of fragmentation). It would be difficult to illustrate this type of uncertainty in a histogram such as Fig. 2 or 5 because the deviation from the “true” age, i.e. the extent of the overcorrection, would depend on the unknown period during which the fragmented surface has had the opportunity to experience alpha ejection. The “true” age would lie anywhere between the corrected date with fragmentation correction (minimum date) and the corrected date without fragmentation correction (maximum date). We could arbitrarily specify a sediment age, for example, and show the resulting histogram, but we think that may be a misleading characterization of the uncertainty, which would depend on geologic constraints specific to a sample. Instead, we propose to add a discussion of this problem, as follows:

Analogous to problem of unknown timing of abrasion for rounded detrital apatite and zircon grains (Rahl et al., 2003; Thomson et al., 2013; Reiners et al., 2018), if the timing of fragmentation is unknown, we could define a maximum date A_{fc}, the FT-corrected date without fragmentation correction, corresponding to fragmentation before or immediately after cooling; and a minimum date A_{ffc}, the fully FT-corrected date with fragmentation correction, corresponding to fragmentation during laboratory mineral separation. If there is sufficient geologic context, we can take the date of the sediment A_s to be the latest time at which the fragmentation occurred, such that the minimum date would be:

$$A_{min} = (A_{ffc}) + (A_{fc}-A_{ffc})(A_s/A_{fc}).$$

A conservative approach would be to display a “plot date” that is the mean of the maximum and minimum possible dates, and an error bar depicting the possible range of dates (Thomson et al., 2013).

In the case of detrital samples for which the timing of fragmentation is unknown, and that have also experienced non-monotonic cooling so that there has been significant diffusive loss after fragmentation (e.g. a fragment in a sedimentary rock that has been partially reset by burial-induced heating), fragmentation-corrected dates will be systematically younger than the corrected dates of whole, unbroken grains. For example, the corrected dates of any whole crystal may reflect a date-Rs relationship, and naively applying the fragmentation correction to fragments will lead to corrected dates that all lie below this the corrected date-Rs relationship of unbroken crystals. In this case, a plot date with a maximum and minimum date could still be calculated, as defined above. The plot dates would reflect a similar date-Rs relationship: i.e. if fragmentation occurred soon after cooling and significantly before partial reheating, the maximum date A_{fc} would be the closest to the corrected date of an equivalent unbroken grain (except that it would be younger than the equivalent unbroken grain to the extent that the unbroken grain is less affected by diffusion due to its size).

In all cases where significant diffusive loss complicates the application of fragmentation correction, the best way to approach the problem may be to consider a combination of factors in deciding whether to apply the fragmentation correction or calculate a plot age that is combination of the fragment-corrected date and the normal FT-corrected date: a.) whether there is a date-size correlation of corrected dates of unbroken grains, and b.) whether the fragment-corrected dates are systematically younger than the corrected dates of unbroken grains, and c.) whether there is geologic context to suspect earlier fragmentation.

One other possible improvement is extending their thinking to the case of modeling: how should a broken grain be entered into thermal history modeling software? Does their reasoning on FT correction also extend to the proper effective radius for diffusion modeling on a sphere? For a grain broken on both sides, an infinite cylinder calculation would probably be the most appropriate, although the proper ejection profile for a cylinder would have to be derived. But, if for now we're stuck with converting everything to a sphere, what is the appropriate conversion?

For the purpose of thermal history modeling (in particular, QTQt, which implements the modelling approach of Brown et al., 2012), apatite helium dates can be input in their uncorrected form, and the fragment dimensions can also be directly entered, without conversion to effective radius. Although Dr. Ketcham's point is certainly valid, because we focus solely on protocols for Ft-corrected dates, we prefer to avoid the considerable additional complexity that would come from discussing thermal history modelling (and the complex additional considerations from timing of breakage on He diffusion effects) in this manuscript.

Regarding the appropriate geometric approximation: the fragmentation correction proposed in the manuscript does not introduce any additional uncertainty that is not already a problem for non-fragments, and potential implications of this for modeling related to this issue have been addressed in the literature (e.g., Gautheron and Tassan-Got, 2010). For consistency, we opted not to introduce a different geometric approximation only for broken grains. Furthermore, because the difference between the beta-FT relationships of various geometric approximations diminishes with lower beta (cf. Fig. 2 of Farley 1996), our proposed correction leads to a slightly smaller difference between the spherical approximation vs. cylindrical/other approximations, compared to the original fragmentation correction.

Regarding the conversion of sphere-equivalent radius for the purpose of evaluating any date- size relationships when fragments are involved, one possibility would be to use the half-width and an assumed aspect ratio for typical crystals to calculate an assumed sphere-equivalent radius (Rs'). Another alternative would be to use a sphere-equivalent radius based on FT (Cooperdock et al., 2019), using the alpha-ejection-affected-FT value proposed here. The rationale would be analogous to the case of the fragmentation FT correction: the alpha-ejection-affected surface-to-volume ratio of a broken crystal is a good proxy for the available-for-diffusion-surface-to-volume ratio.

Finally, if the broken grain boundary is inclined with respect to the c-axis rather than perpendicular, what is the appropriate length – the long edge along the c-axis, the short edge along the c-axis, or their average (which is roughly equivalent to the length along a central axis, a reasonable estimate for the axis of symmetry)? In most cases, it probably amounts to a negligible difference, but for the sake of completeness it would be good to consider and discuss.

Because fragmentation of apatite is almost always along a crystallographically controlled cleavage, it is uncommon to see obliquely broken fragments. In the rare cases of such fragments, the appropriate length measurement to use would simply be the length along the central axis. i.e. assuming that the crystal is symmetrical with respect to the c-axis, an obliquely fragmented crystal of average length 85 um (e.g. long edge 90um, short edge 80um) would have exactly the same fraction of helium retained as a perpendicularly fragmented crystal of length 85 um.

We will clarify this in the revised manuscript.

[line 30] Delete "both"

[line 93-94] Delete "since the widespread application of the technique"

[line 296] Does this sentence refer to the error bars? Maybe better to say it directly: "Error bars in date-elevation profile represent dispersion of dates corrected with new protocol only."

[line 333] Spell out XRCT

We agree with the above four line-by-line comments and will revise as suggested.