Supplemental Material

Tectonic origin of the Great Unconformities of the Rocky Mountain region: the power of combined zircon (U/Th)-He and K-feldspar $^{40}\text{Ar}/^{39}\text{Ar}$ thermochronology

Here we provide full descriptions of the newly presented data and modeling procedures. This document contains the following figures and tables:

Figs. DR1-5 – Plots of $^{40}\text{Ar}/^{39}\text{Ar}$ K-feldspar data

Fig. DR6 – Sample-specific forward models for each location

Fig. DR7 – Increasingly constrained Los Pinos inverse models

Fig. DR8 – Inverse models testing the possibility of Proterozoic reburial

Table DR1 – $^{40}\text{Ar}/^{39}\text{Ar}$ K-feldspar sample locations

Table DR2 – $^{40}\text{Ar}/^{39}\text{Ar}$ K-feldspar analytical data

Table DR3 – New ZHe data

Table DR4 – Complete inverse modeling inputs, assumptions, and modeling parameters, following methods outlined in Flowers et al. (2015).

$^{40}\text{Ar}/^{39}\text{Ar}$ K-FELDSPAR METHODS AND DATA

The K-feldspar multiple diffusion domain (MDD) analytical methods follow those presented in detail in Sanders et al. (2006) with additional details presented here for the 4 used in this study. The samples were irradiated in machined Al disks in either the 5C position at the McMaster University reactor, Ontario, for 52.8 MW hours (irradiation NM-145), 54.0 MW hours (irradiation NM-188), and 86.0 MW hours (irradiation NM-122) or the central thimble at the USGS Denver reactor (40 MW hours, NM-254). Neutron flux gradients were measured using Fish Canyon sanidine placed in holes of known geometry in the Al disks. All ages and J-factors are calculated using Fish Canyon at 28.201 Ma (Kuiper et al., 2008) and a total ^{40}K decay constant of $5.463\text{e-}10$ /a (Min et al., 2000). Typically, 4 single crystals from each position were analyzed to determine the J-value. Mean values for each location were fit with a sine curve and J-values for unknowns were extrapolated based on their geometric relation. J-factor errors are determined at 0.1 to 0.2% (1σ). Correction factors for interfering reactions were

measured using CaF_2 and K-glass included with the samples during irradiation. The correction factors are given in the footnotes of the data tables.

Samples were step heated in a double vacuum molybdenum resistance furnace. K-feldspar separates (generally a single fragment) wrapped in Cu-foil were heated with high resolution (31-42 steps) heating schedules, and isothermal replicate steps were conducted to help evaluate excess argon contamination (e.g. Harrison et al., 1993). For samples other than Vestegard, the gas released was reacted with a SAES GP-50 getter operating at $\sim 450^\circ\text{C}$ during heating followed by a second stage of clean up using 2 SAES GP-50 getters (one at 20°C , one at $\sim 450^\circ\text{C}$) and a tungsten filament operated at $\sim 2000^\circ\text{C}$. The gas was typically gettered for 2 minutes in the second stage. These samples were analyzed on an MAP-215-50 mass spectrometer. The Vestegard sample was cleaned during heating with a cold GP-50 during heating and additionally reacted in a $\sim 450^\circ\text{C}$ GP-50 in a second stage for 60 seconds before isotope analysis using a Thermo Scientific Helix MC mass spectrometer. The furnace thermocouple was calibrated by melting Cu-foil and true furnace temperature was 35 or 50°C lower than the thermocouple temperature. Heating schedules were adjusted by this amount, and corrected sample temperatures are reported in data tables.

Furnace blank and background values were determined by running a 15 minute, 800°C hot blank prior to each analysis. Blank values range between 600-800, 7-15, 0.7-0.9, 6-8, and $2.8\text{--}3.3 \times 10^{-18}$ moles for masses 40, 39, 38, 37, and 36, respectively. For these high K and old samples, blank corrections are commonly insignificant.

The MDD thermal histories were obtained using the basic procedures of Lovera et al. (1989) and Sanders et al. (2006). The MDD data are plotted in supplemental figures DR1-DR5 showing measured and modeled age spectra (a), Arrhenius data (b), $\log(r/r_0)$ plots (c) and thermal history plots (d). Diffusion coefficients are calculated based on the fractional release of ^{39}Ar and plotted on Arrhenius plots. $\log(r/r_0)$ plots were obtained by using an activation energy of 46 kcal/mol (Lovera et al., 1997) and using the convention of placing the reference Arrhenius law (r_0) to pass through the first heating step such that the $\log(r/r_0)$ value is zero for the first increment of gas release. The $\log(r/r_0)$ plots have a form consistent with a multi-domain behavior with inflections that closely correlate to inflections within the age spectra. The Arrhenius data were

forward modeled with activation energy for each domain of 46 kcal/mol and a domain distribution that utilizes 5 to 7 domains to yield model fits that closely match the measured data. Fitting the measured age spectrum with acceptable fits determined by a Chebyshev's approximation derives the model thermal histories. A minimum of 20 successful model fits is used to determine a mean and 90% confidence interval for the thermal histories that only allow cooling from and initially high temperature (brown and yellow polygons). Due to the post Precambrian heating related to Phanerozoic burial, the cooling only thermal histories are not geologically consistent, however the intent is to derive a segment of the Precambrian thermal history that is resultant from cooling only. The measured age spectra can also be well modeled with unconstrained thermal histories (grey lines). These models generally coincide with the cooling only models for the high-temperature history and also show that many paths can be used to produce the minor argon loss observed in the Phanerozoic. However, in all cases the samples reached ~150-175°C in the late Mesozoic- early Cenozoic and thus are consistent with the geological burial history and ZHe models.

Also included are several forward models that simulate the high temperature Precambrian thermal history for cooling only and then model the samples coming to the surface at different times in the Precambrian followed by various Phanerozoic burial/heating histories. For instance, the Long's Peak sample can be exhumed in the Precambrian at a variety of different times and as early as 900 Ma followed by the requirement of heating to ~175°C by about 75 Ma. In contrast, the Los Pinos sample is required to still be hot (>200°C) at 900 Ma and can only reach the surface after 700 Ma. Taken together, the K-feldspars, like the ZHe data show variable thermal histories within the Rocky Mountain region.

THERMAL HISTORY MODELING

Forward Modeling

Forward modeling efforts use the zircon radiation damage and annealing model (ZrDAAM) of Guenthner et al. (2013). The generalized forward models presented in Figure 2 are not meant to represent any single sample location, but instead provide a basic thermal history of the Rocky Mountain region. These models begin at a crystallization age of 1700 Ma, representative of rocks within the Yavapai Province

(Whitmeyer and Karlstrom, 2007). Younger rocks of the Mazatzal Province (1650-1600 Ma) would yield identical forward modeling results, and are not modeled. Forward models also include a 350 °C temperature constraint at 1400 Ma, based on a regional investigation of the cooling history of the southern Rocky Mountains using $^{40}\text{Ar}/^{39}\text{Ar}$ hornblende, muscovite, and biotite cooling ages of rocks south of the Cheyenne Belt (Shaw et al., 2005). Forward models are also forced to surface temperatures between 550-310 Ma based on the range of overlying Paleozoic strata across the Rocky Mountains. Finally, forward models are buried to maximum temperatures of 125 °C at 80 Ma to simulate deposition of Paleozoic and Mesozoic strata prior to Laramide exhumation.

Sample-specific forward models using existing constraints are presented in Figure DR6, and include available geochronologic, thermochronologic, and geologic constraints for each sample location. These models were constructed to test how compatible ZHe datasets are with additional constraints, including K-feldspar data. Including additional $^{40}\text{Ar}/^{39}\text{Ar}$ thermochronologic data, specifically K-feldspar constraints, limits the plausible times that each sample can cool to the surface, and each forward model tests a range of different cooling paths. However, these paths are designed to coincide with known geologic events, including 1300-900 Ma assembly and 770-570 Ma break-up of Rodinia (Yonkee et al., 2014), 717-635 Ma Snowball Earth (Rooney et al., 2014), and 350-300 Ma Ancestral Rocky Mountain deformation. While ZHe date-eU curves are highly dependent on radiation damage within each crystal (Guenther et al., 2013), they may also be influenced by differences in crystal size. To include these possible effects, we model three separate ZHe date-eU curves to create an envelope, similar to previous workers (e.g. Orme et al., 2016; DeLucia et al., 2017; Ault et al., 2018; Reade et al., 2020). To create the three curves, we use the mean grain size ± 1 standard deviation. Resulting forward models are then compared to ZHe data from each sample. ZHe data is presented in Table DR3. A complete description of model constraints is included in Table DR4.

Sample-specific forward modeling results show that the inclusion of K-feldspar constraint boxes drastically limits the possible times of rapid cooling to near-surface temperatures. All samples show similar slopes in the resulting ZHe date-eU curves. The

largest difference between early cooling and late cooling in each sample is the maximum ZHe date at low eU values, which can vary by several hundred million years (Fig. DR6). These results are useful for testing the compatibility between ZHe data and K-feldspar data. Differences in the resulting ZHe date-eU curve for each sample also show that ZHe data are also sensitive to the Proterozoic thermal history, and that combining ZHe with K-feldspar data will result in a better constrained model than either dataset separately. All forward models, however, fail to predict ZHe date-eU curves that match the observed data, suggesting that these overly simplistic scenarios fail to account for the geologically complex history these samples have experienced. Inverse modeling provides the ability to test more complex cooling paths.

Inverse Modeling

HeFTy v. 1.9.3 (Ketcham, 2005) was used for inverse modeling of ZHe data to explore viable thermal histories for each sample. Our modeling efforts were constructed to test two main parameters: 1) Whether ZHe datasets are compatible with other geochronologic, thermochronologic, and geologic constraints, and 2) Whether ZHe datasets add additional constraints to a sample's thermal history. To do this, we included multiple user-defined constraint boxes that forced the sample through a particular time-temperature space. These constraint boxes are fully described in Table DR4. HeFTy limits the number of input grains to 7, so samples that have more than 7 ZHe dates were binned to create synthetic grains. Each input grain included 15% grain date uncertainty.

The Boulder Creek model yielded a total of 185 acceptable and 71 good paths (Fig. 4). $^{40}\text{Ar}/^{39}\text{Ar}$ K-feldspar MDD modeling indicates that this sample cooled relatively rapidly from 300-200 °C between about 1250-1100 Ma (Figs. 3, 4). The ZHe inverse models show a wide range of cooling below 100 °C from ca. 1190-520 Ma, with pulses of rapid cooling during the same period.

The Tusas Mountains model yielded 93 acceptable and 30 good paths (Fig. 4). This sample cooled to 350 °C at ca. 1350 Ma, constrained by $^{40}\text{Ar}/^{39}\text{Ar}$ muscovite data (Shaw et al., 2005). $^{40}\text{Ar}/^{39}\text{Ar}$ biotite cooling ages are all older than 1294 Ma (Shaw et al., 2005) such that this region must have cooled below ~275 °C at that time (Fig. 4).

ZHe data constrain the sample to >200 °C until 600 Ma, followed by rapid exhumation to near-surface temperatures between 520 and 310 Ma.

The Santa Fe Range model resulted in a total of 47 acceptable and 1 good paths (Fig. 4). $^{40}\text{Ar}/^{39}\text{Ar}$ muscovite data suggest this sample was at 350 °C at 1372 Ma and MDD K-feldspar thermal models (Fig. 3) show that this sample remained >150 °C until 700-600 Ma (Sanders et al., 2006). In the final inverse model, good path segments with cooling rates >10 °C/Ma show rapid cooling during assembly of Rodinia, during which time the sample cooled to minimum temperatures of ~100 °C, followed by final cooling younger than 800 Ma.

The Sandia Mountains model resulted in a total of 11 acceptable and 1 good paths (Fig. 4). This sample cooled to <350 °C soon after crystallization based on $^{40}\text{Ar}/^{39}\text{Ar}$ muscovite ages (Sanders et al., 2006) and resided above ~250 °C until about 1150 Ma before cooling to ~175 °C by 900 Ma (Fig. 3). Final cooling may have occurred during an earlier timeframe (850-750 Ma), or alternatively during a younger pulse from 520-350 Ma).

The Los Pinos Mountains model resulted in a total of 7 acceptable and 0 good paths. K-feldspar MDD thermal models indicate this sample was above ~275 °C until 950 Ma and cooled through 175 °C by 700 Ma (Fig. 3). At temperatures lower than 150 °C (the lower limit of K-feldspar sensitivity), this sample shows multiple discrete pulses of cooling, with final cooling to near-surface temperatures occurring after snowball Earth. This sample was also used to construct a series of inverse models that highlight the “seesaw” effect in modeling ZHe data (Fig. DR7). As additional constraint boxes are added during inverse modeling, the final models become tighter constrained at segments of the cooling path that are far removed from the input box, and also sometimes allows for more paths to be found.

Figure DR8 shows inverse models for each sample that test for the possibility of Proterozoic reburial. All models are compatible with monotonic Proterozoic cooling (Fig. 4), and none of the sample locations preserves any geologic evidence or Proterozoic reburial, such as Proterozoic sedimentary deposits. However, it is possible that Proterozoic sedimentary deposits may have existed, and were completely removed by erosion prior to formation of the Great Unconformity. To test the compatibility of ZHe

data with this hypothesis, Figure DR8 presents inverse models that force the sample to cool immediately after K-feldspar constrain boxes. Each model is then allowed, but not required, to experience a pulse of reheating to maximum possible temperatures of 300 °C, followed by cooling back to surface temperatures. Since “good” and “acceptable” paths are found with monotonic cooling scenarios (Fig. 4), none of the samples require reheating; However all samples are permissive of this scenario (Fig. DR8).

SUPPLEMENTARY FIGURES AND TABLES

Figure DR1. MDD data for Boulder Creek sample. **A.** Measured and modeled age spectra **B.** Arrhenius data **C.** $\log(r/r_0)$ plots, and **D.** Thermal history plots. Different colored lines represent different cooling paths that are modeled.

Tusas, NM
Vestegard

Figure DR2. MDD data for Tusas Mountains sample. **A.** Measured and modeled age spectra **B.** Arrhenius data **C.** $\log(r/r_0)$ plots, and **D.** Thermal history plots. Different colored lines represent different cooling paths that are modeled.

Figure DR3. MDD data for Santa Fe sample. **A.** Measured and modeled age spectra **B.** Arrhenius data **C.** $\log(r/r_0)$ plots, and **D.** Thermal history plots. Different colored lines represent different cooling paths that are modeled.

Sandia granite
SAN-03-02

Figure DR4. MDD data for Sandia sample. **A.** Measured and modeled age spectra **B.** Arrhenius data **C.** $\log(r/r_0)$ plots, and **D.** Thermal history plots. Different colored lines represent different cooling paths that are modeled.

Figure DR5. MDD data for Los Pinos sample. **A.** Measured and modeled age spectra **B.** Arrhenius data **C.** $\log(r/r_0)$ plots, and **D.** Thermal history plots. Different colored lines represent different cooling paths that are modeled.

Figure DR6. Sample-specific forward models for each of the 5 locations and resulting ZHe date-eU curves and envelopes. Forward model constraints are described in Table DR2, and include all available geologic, thermochronologic, and geochronologic constraints available. Grain sizes are averages of all grains per sample, with 1σ standard deviation. All samples include new K-feldspar constraint boxes, and show how these data help to further constrain the thermal history. When K-feldspar data are included, the ZHe data show much less variability in the resulting date-eU curves. 1 = assembly of Rodinia; 2 = break-up of Rodinia; 3 = snowball Earth; 4 = Ancestral Rocky Mountains; 5 = Laramide orogeny; 6 = Neogene exhumation.

Figure DR7. Los Pinos inverse models showing the effect of progressively adding constraint boxes to help guide the model.

Figure DR8. Inverse models for each sample location testing the hypothesis that samples were cooled to surface temperatures during the Proterozoic, followed by a period of reburial and cooling to form the Great Unconformity. Each model assumes rapid cooling to surface temperatures immediately after the K-feldspar constraints. Reburial boxes allow for the possibility of no reburial and reach maximum temperatures of 300 °C. **A.** The Boulder Creek model allows for a range of reburial maximum temperatures, although some paths indicate no reburial. **B.** All good paths, and most acceptable paths, for the Tusas Mountains require some amount of reheating. However, these paths show maximum reburial temperatures >200 °C to completely reset ZHe data. If true, this would indicate an unrealistically thick sedimentary basin that has since been completely removed by erosion. Instead, a simpler interpretation is that the sample remained at higher temperatures until post-500 Ma cooling. **C.** Some paths for the Santa Fe model show some amount of reheating, but others indicate no reheating. **D.** The Sandia Mountains model is also compatible with both scenarios, including varying amounts of reheating and no reheating. **E.** The Los Pinos model only yielded 2 acceptable paths, making interpretations tenuous. However, they both indicate some amount of reheating, suggesting that this dataset may also be compatible with this scenarios as well as monotonic cooling during the Proterozoic.

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