



Cluster analysis on a sphere: Application to magnetizations from metasediments of the Jack Hills, Western Australia

Richard K. Bono^{a,*}, John A. Tarduno^{a,b}, Matthew S. Dare^a, Gautam Mitra^a, Rory D. Cottrell^a

^a Department of Earth and Environmental Sciences, University of Rochester, Rochester, NY 14627, United States

^b Department of Physics and Astronomy, University of Rochester, Rochester, NY 14627, United States

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ABSTRACT

Metasediments of the Jack Hills contain the oldest known terrestrial minerals in the form of zircons nearly 4.4 billion years old. Paleointensity data from these zircons provide evidence for a Hadean geodynamo as old as 4.2 billion years old. Given the importance of these zircons for constraining the earliest history of the core, it is vital to understand the fidelity of the zircon record. A fundamental aspect providing context for the preservation of primary magnetic signals is the nature of overprints predicted to have been imparted on rocks of the Jack Hills due to Archean to Proterozoic metamorphic events. To be viable magnetic records of a Hadean geodynamo, zircon magnetization directions should differ from these secondary magnetizations. To evaluate these secondary magnetizations, we report paleomagnetic analyses of a comprehensive sampling of 68 quartzite cobble-sized clasts from the Jack Hills metasediments ~0.5 to 1.0 km from the Discovery Site (which has yielded the oldest zircons and paleofield estimates). While application of standard paleomagnetic tests suggests that the ensemble of cobble directions cannot be distinguished from those drawn from a random distribution, a new cluster analysis of directions on a sphere and non-parametric resampling approaches reveal significant directions amongst subsets of the data. One, isolated at the lowest temperature analyzed [200 to 300 °C, Declination (Dec.) = 316.8°, Inclination (Inc.) = −51.1°] appears to be dominated by the present day field. Another, isolated at higher (but still relatively low unblocking temperatures that we call “intermediate”, of ~350–500 °C, Dec. = 243.8°, Inc. = 9.5°) agrees with a magnetic overprint isolated from the secondary Cr–Fe mica fuchsite isolated from the Jack Hills Discovery site, passing a field test at the 80% confidence level. No evidence is found in our data, or in the data of others collected on similar Jack Hills lithologies, for a widespread 1 Ga remagnetization event. Instead, we interpret the most prevalent secondary magnetization of the quartzite (i.e., intermediate unblocking) and the fuchsite characteristic remanent magnetization to be ~2.65 Ga in age, coincident with peak metamorphism (as high as ca. 475 °C) of the Jack Hills. The presence of this distinct secondary magnetization, its difference from that recorded by Jack Hills zircons at high unblocking temperatures, and the lack of a dominant remagnetization direction at high unblocking temperatures in the cobble data (the expected result for a primary magnetization), lends further support to the fidelity of the Hadean geomagnetic record. The presence of the secondary magnetization also lends support to the conclusion that most of the Jack Hills metasediments were deposited in the Archean, with only minor reworking and potential tectonic interleaving of Proterozoic components. Overall, the application of the new directional cluster analysis presented here has the potential to reveal magnetic directions in highly scattered data sets, typical of weakly magnetized coarse-grained sedimentary rocks.

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1. Introduction

Metasediments of the Jack Hills contain the oldest known terrestrial minerals in the form of zircons nearly 4.4 billion years old (Wilde et al., 2001; Valley et al., 2014). Paleointensity data from these zircons provide evidence for a Hadean geodynamo

as old as 4.2 billion years old (Tarduno et al., 2015). A positive microconglomerate test conducted on 500 to 800 μm samples from oriented thin sections each centered on a large 200–300 μm zircon indicates that the zircons retain magnetizations at very high unblocking temperatures (ca. 550–580 °C), escaping remagnetization by later geological events. This conclusion is consistent with the peak metamorphic temperatures of ca. 475 °C (Rasmussen et al., 2010, 2011). Further support has been provided

* Corresponding author.

E-mail address: richard.bono@rochester.edu (R.K. Bono).

by recent documentation of the preservation of Li zonation in a zircon (Trail et al., 2016) that suggests the key Jack Hills Discovery site (also known as W74), from which the zircons yielding Hadean ages and magnetizations reported in Tarduno et al. (2015) were obtained, has not experienced amphibolite grade metamorphism (specifically, temperatures greater than 500 °C) since deposition.

While the microconglomerate test excludes chemical and thermal remagnetization of high unblocking temperature magnetizations (Tarduno et al., 2015), it is nevertheless useful to understand the magnetic overprinting history of the Jack Hills metasediments. In addition to providing further context for the zircon magnetizations, this history can provide clues to the tectonic evolution of the Jack Hills (Cottrell et al., 2016).

On the basis of the study of cobble-sized quartzite clasts from the Jack Hills (the first paleomagnetic study of the Jack Hills), Tarduno and Cottrell (2013) concluded that at highest unblocking temperatures, generally greater than 550 °C, a component of magnetization is present that cannot be distinguished from a random distribution using the classic test of Watson (1956). This was the first indication that the Jack Hills sediments might preserve a primary magnetization. The presence of a high unblocking temperature component in samples from the Tarduno and Cottrell (2013) collection was confirmed by independent measurements in a second laboratory [Lehigh University, reported in Dare et al. (2016)]. Remagnetization at ca. 1 Ga was first discussed by Tarduno and Cottrell (2013) but rejected because of the lack of directional evidence. Tarduno and Cottrell (2013) also observed a shallow magnetization at intermediate unblocking temperatures (300–500 °C), but this was observed in only about 20% of the samples (28 cobbles were analyzed).

To better isolate the remagnetization history, Cottrell et al. (2016) sampled fuchsite, a secondary chrome mica from the Discovery Site. Fuchsite grains commonly contain relict Cr–Fe spinels capable of recording magnetizations at unblocking temperatures that should have been reset by peak metamorphic conditions. Indeed, the fuchsite was found to record a well-defined magnetization between ca. 270 and 340 °C that was interpreted to record the geomagnetic field as viewed from the Yilgarn Craton at ca. 2.65 Ga, imparted during peak metamorphic reheating.

Herein, we revisit the question of low to intermediate unblocking temperature magnetizations recorded by the cobble-sized cobbles of the Jack Hills. To determine whether a larger sample set might reveal a more coherent pattern of overprint, the initial 28 samples of Tarduno and Cottrell (2013) were supplemented by the collection of 40 new cobbles. We present new thermal demagnetization results, and subsequent analyses.

The high degree of directional scatter motivated the development of a new method of analysis of directional data on a sphere. This new approach reveals directions that are not obvious from application of the iconic randomness tests of Watson (1956). Specifically, the direction of magnetization recorded by the fuchsite of the Discovery site is also present at intermediate unblocking temperatures in the Jack Hills cobbles. This indicates that the most important overprint direction in the Jack Hills sediments is that carried by the fuchsite and the intermediate unblocking temperature component of the Jack Hills cobbles, possibly imparted at ~2.65 Ga. The difference between this magnetic direction and directions isolated at high temperatures from oriented single zircons yields further support for select Jack Hills zircons as magnetic recorders and the presence of a Hadean geomagnetic field (Tarduno et al., 2015). The isolation of this ancient remagnetization direction at the Discovery Site and in a long transect of cobble-bearing sediments supports the conclusion that most of the Jack Hills metasediments have Archean depositional ages, with only

minor reworking and possible tectonic interleaving of younger Proterozoic components.

2. Field collection and sampling

Quartzite cobbles were sampled from the same horizon reported on by Tarduno and Cottrell (2013) in 2012 as part of a long term study of the magnetic component structure of these rocks and magnetic provenance (Fig. 1; Supplementary Fig. SM1.1 and Table SM1.1), representing the graduate thesis studies of M.S. Dare and R.K. Bono. Procedures follow those of Tarduno and Cottrell (2013) with the following revisions. Tarduno and Cottrell (2013) focused on cobbles with a minimum of flattening with the reasoning that these cobbles would have undergone rolling, minimizing penetrative deformation (Ramsay and Huber, 1987). To increase the sample size, some more flattened cobbles were sampled, and beds off strike from the Tarduno and Cottrell (2013) were sampled. In addition, to increase the diversity of clasts as part of a study of magnetic provenance (Dare et al., 2016), a few irregularly shaped clasts having sedimentary banding were sampled. Laboratory sampling of each cobble follows procedures outlined in Tarduno and Cottrell (2013). Cobbles were split using diamond saws and the interior of each was inspected to find an optimal location (least recrystallization and weathering) for an ~3–6 cc cube (~10 g) for paleomagnetic analysis (see Supplementary Fig. SM1.2). A photographic catalog of every field sample (except JC23 and JC24 where laboratory photographs are provided in lieu of field photographs, which were not taken because of low light) for this study and that of Tarduno and Cottrell (2013) is provided in Supplementary Materials SM2.

3. Thermal demagnetization

Thermal demagnetization experiments were conducted in air using a magnetically shielded (~10 nT), ASC Scientific Thermal Demagnetizing Oven (TD-48), heating samples in a step-wise fashion from 100 to 600 °C, typically in 25 °C increments. For each temperature step, sample order within the demagnetizing oven was preserved; samples were rotated 180° between each step in the oven. Paleomagnetic measurements were done using a liquid helium cooled 2G Enterprises 3-component DC SQUID (model 755) magnetometer at the University of Rochester, which is equipped with high resolution sensing coils and a 4.2 cm room-temperature access bore. The 4.2 cm access bore is necessary to accommodate samples that are large enough to bear sufficient magnetic material. This ensures that the SQUID magnetometer can reliably measure the magnetically weak, bulk sedimentary rock samples [see Dare et al. (2016), for more discussion on SQUID magnetometer sensing limitations]. The demagnetizing oven and magnetometer are housed within a magnetically shielded room with an ambient magnetic field of <200 nT.

4. Analyses

4.1. Temperature intervals and principal component fits

We follow the nomenclature outlined in Tarduno and Cottrell (2013) for assigning unblocking ranges, with “low” temperature, LT, (typically between 200–300 °C, $n = 46$), “intermediate” temperature, IT, (~350–500 °C, $n = 55$), and “high” temperature, HT, (~550–580 °C, $n = 54$) unblocking temperature components (Fig. 2). Six cobbles with smooth, linear decay trends were interpreted to record lightning strikes and excluded from further analysis. Select unblocking components have been reported previously in Tarduno and Cottrell (2013) and Dare et al. (2016). A summary of the LT, IT and HT unblocking components is presented

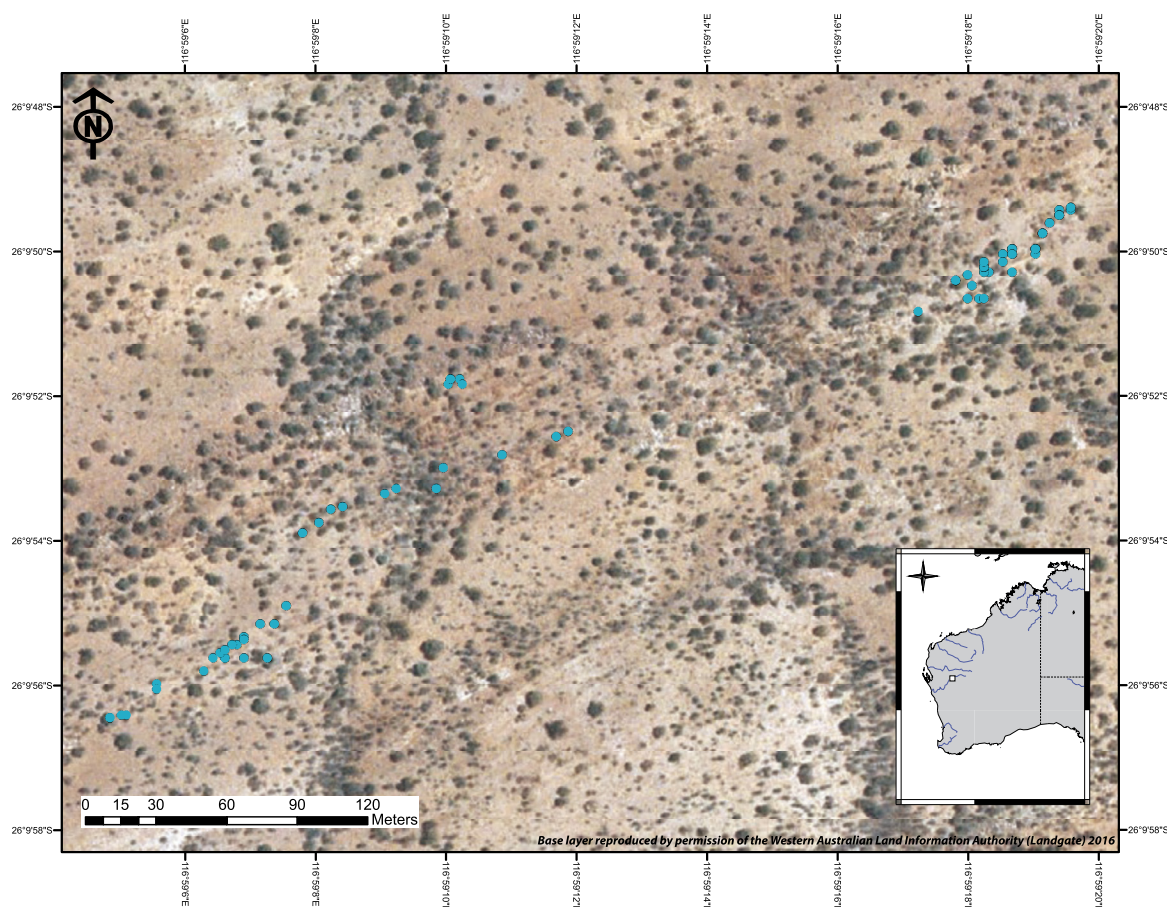


Fig. 1. Location of Jack Hills (Western Australia) cobble sampling. Inset: location of Jack Hills. See Supplementary Fig. SM1.1 for detailed sampling map.

in Fig. 3 and Supplementary Tables SM1.2–SM1.4. Principal component analysis was performed to identify unblocking component directions; we require principal components to include at least three measurement steps and have a maximum angle of deviation (MAD) of less than 25° (in all but two unblocking components, the MAD angle was less than 20°). Thirty-nine of 54 ($\sim 72\%$) of HT unblocking components trend closely to the origin in orthogonal vector plots and hence the origin was included in the calculation of the characteristic remanence magnetization direction (Supplementary Table SM1.4). Deviation from the origin for the other samples likely reflect the presence of some minor hematite related to modern weathering.

4.2. Watson randomness tests

The LT unblocking components are highly scattered and when a Watson (1956) test for randomness is performed, the set of directions fails to pass ($R = 7.48$, $R_0 = 10.91$, $n = 46$). In this test, the resultant vector, R , of the Fisher mean for the set of directions (Fisher, 1953) is compared to a critical threshold, R_0 for a given probability. If R does not exceed R_0 , then the null hypothesis (of randomness) cannot be rejected at the assigned confidence level (95%). Similar tests were performed on the IT and HT unblocking components (IT: $R = 7.59$, $R_0 = 11.93$, $n = 55$; HT: $R = 5.29$, $R_0 = 11.82$, $n = 54$); the null hypothesis was unable to be rejected for these higher unblocking temperature datasets as well. The highest unblocking temperature component generally trends to the origin of orthogonal vector plots. This, together with its linearity, favors the standard interpretation that this component was acquired prior to the deposition of the host conglomerate unit (Tarduno and Cottrell, 2013). We note that a high temperature magne-

tization has been observed in all studies of the Jack Hills cobbles, but with differing degrees of resolution (Supplementary Materials SM1). But the lower unblocking temperature magnetizations (LT and IT), which cannot be primary, also appear to have a random distribution following the application of the Watson (1956) test.

Partial thermoremanent magnetization experiments (Supplementary Materials SM3) show that some of cobbles are capable of recording thermal overprints, but with scatter that is likely related to their complex magnetic mineralogy (containing in varying amounts magnetite, Cr-Fe spinels, hexagonal pyrrhotite, monoclinic pyrrhotite, titanohematite, and various oxidized forms including maghemite and hematite), grain size distributions, possible anisotropy (Dare et al., 2016) and in some cases, a potentially insufficient number of magnetic grains (Berndt et al., 2016). As we demonstrate below, the standard Watson (1956) test is not suitable for the detection of a coherent direction represented by a subset of an overall dataset with high scatter that might possibly record the expected low to intermediate temperature overprinting of the Jack Hills sediments.

4.3. Cluster analyses on a sphere

To address the challenge of recognizing possible magnetic directions retained within a subset of the nominally randomly distributed data, a method was developed to detect possible clusters of coherent directions. Contour analysis of paleomagnetic data requires special consideration not typically employed in other geologic studies to account for the full range of paleomagnetic directions (i.e., since inclination can be either positive or negative, a full sphere needs to be explored). Common software tools for contouring geologic data [e.g., Stereonet 9, Allmendinger et al. (2012)]

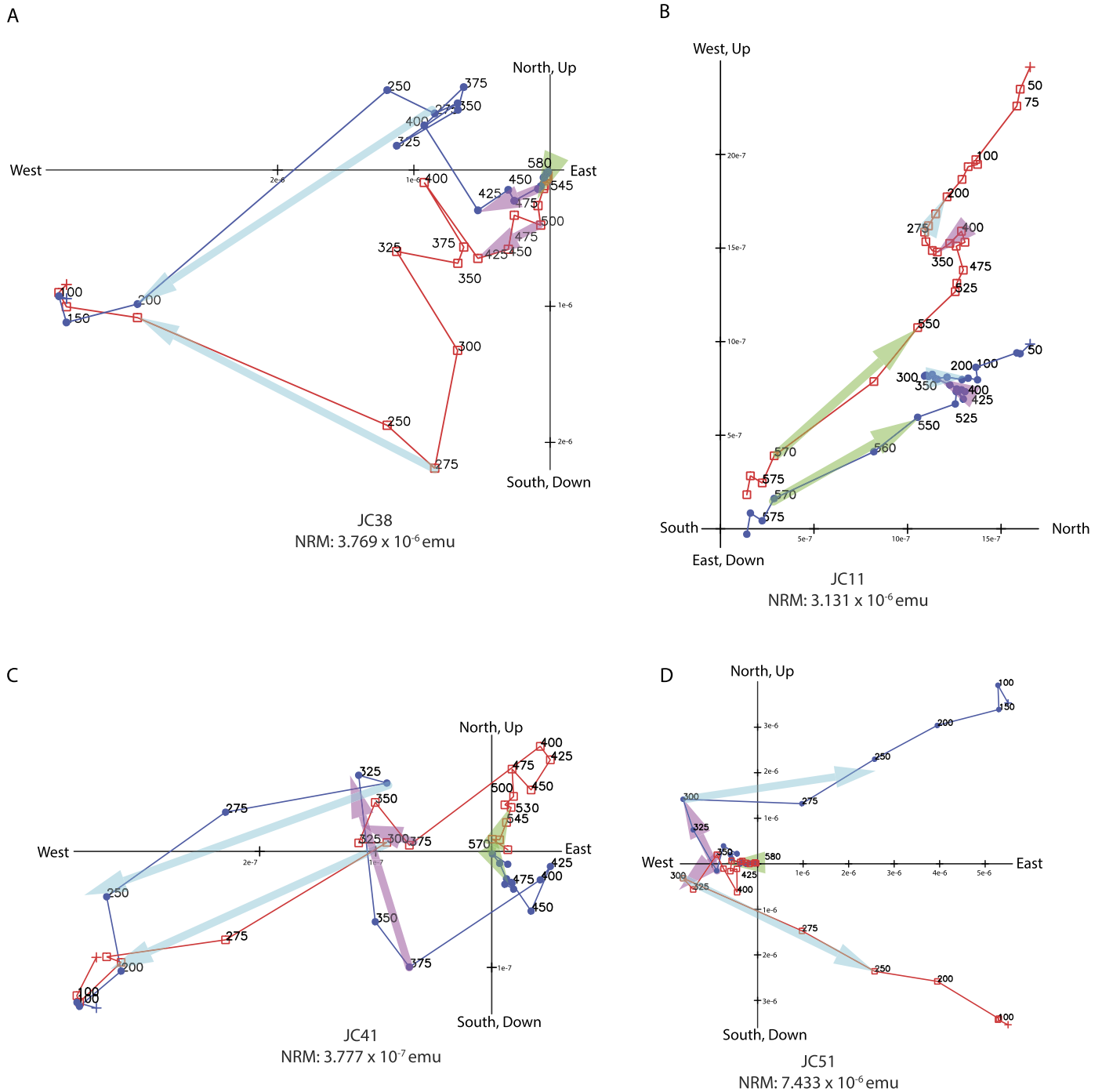


Fig. 2. Orthogonal vector plots of thermal demagnetization experiments in geographic coordinates. Red squares, stereonet projection of the vertical component of magnetization; blue circles, declination. Arrows show assigned unblocking temperature components: blue, low temperatures (LT); red, intermediate temperatures (IT) and green, high temperatures (HT). A) Sample JC38. B) Sample JC11. C) Sample JC41. D) Sample JC51.

do not make this distinction. Here, we define a regular counting grid with 5° spacing over a declination range of -180° to 175° (to avoid duplicate counts where longitude = $-180/180^\circ$) and an inclination range of -90° to 90° . For each grid node, all paleomagnetic directions within a constant distance are counted (counting circle radius, $\sim 36^\circ$, comprises an area containing about 10% of a sphere's surface).

Independent of the spherical contouring presentation, paleomagnetic directions (in Cartesian coordinates) underwent cluster analysis. Three methods were employed to determine cluster grouping and centers: k-means clustering (Hartigan, 1972), fuzzy

c-means clustering (Dunn, 1973; Bezdek, 1981) and Gaussian mixture models (Figueiredo and Jain, 2002). These k-means and fuzzy c-means clustering returned similar results but the former generally agreed better with the spherical contour analysis. In some cases there was disagreement between analyses leading us to suspect the presence of artifacts (see Section 5).

In k-means clustering, n directions are grouped into a predefined number of clusters, k , wherein each direction belongs to the cluster with the closest mean direction. In our application, the number of clusters, k , was incremented from 1 to n , the number of directions in the data set. To select the appropriate k clusters

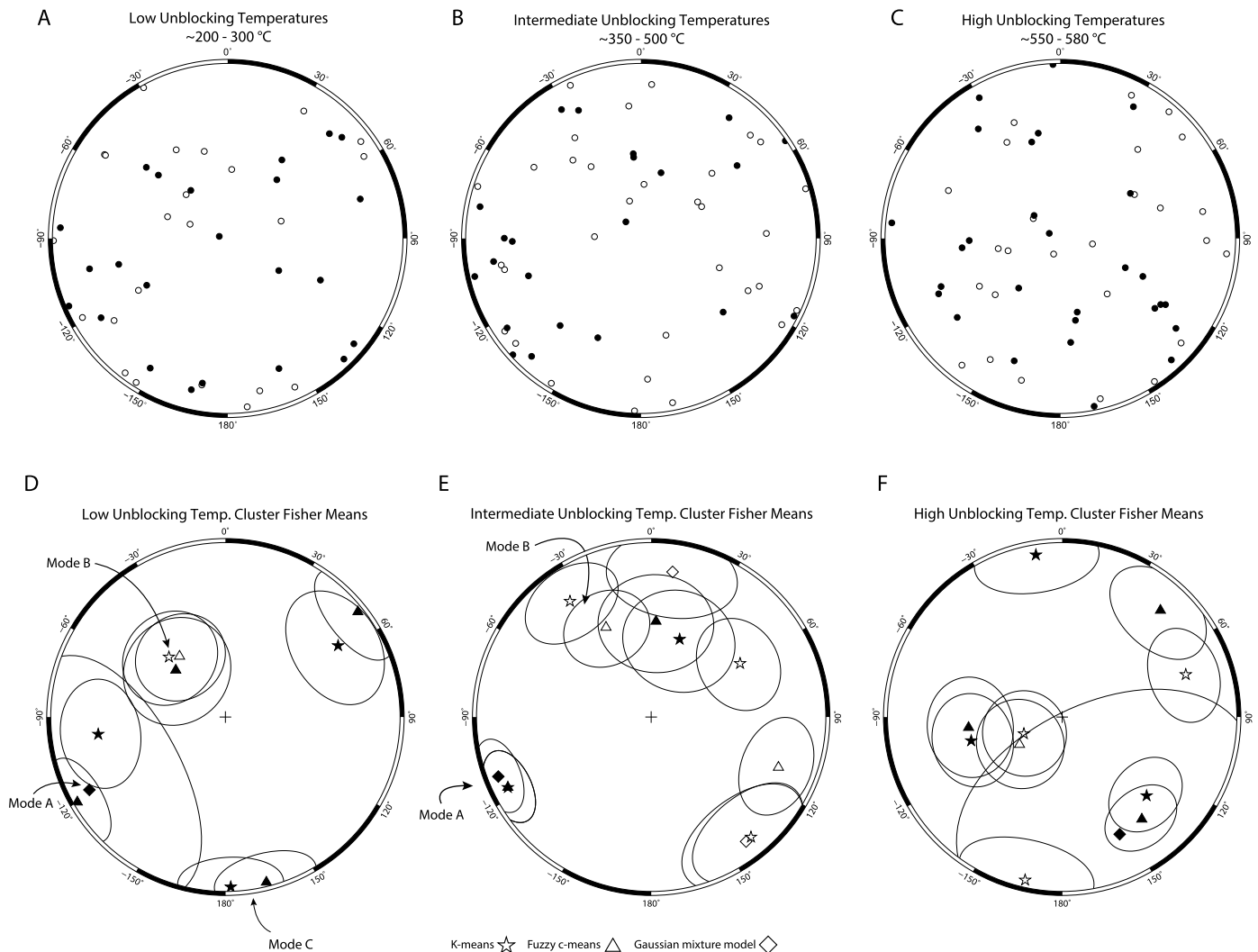


Fig. 3. Equal area stereonet showing directions for assigned unblocking temperature components. Open symbols, negative inclinations; solid symbols, positive inclinations. A) Low temperature (LT) unblocking components; B) Intermediate temperature (IT); C) High temperature (HT). D) Equal area stereonet showing Fisher mean directions with 95% confidence intervals from cluster analyses for LT components. Open symbols, negative inclinations; solid symbols, positive inclinations. Star: *k*-means clustering; triangle: fuzzy *c*-means clustering; diamond: Gaussian mixture model clustering. E) IT components, following (D). F) HT components, following (D).

that best describe the data, the mean silhouette value (Kaufman and Rousseeuw, 2005) was determined for each iteration. Silhouette values describe how distant a given direction in one cluster is to directions in neighboring clusters, where a value +1 describes a direction that is distant from all neighboring clusters, 0 describes a direction whose cluster assignment is indistinct, and −1 implies the direction is possibly assigned to an inappropriate cluster. The mean silhouette value for all directions can be used as a proxy for how well *k* clusters separate directions into distinct groups. To avoid over-fitting the directions into too many clusters, the *k* corresponding with the lowest order local maximum in mean silhouette value was chosen.

Fuzzy *c*-means clustering is similar to the *k*-means approach, except that for each direction the degree to which it belongs to each cluster is also determined (termed “membership”), allowing for a direction to potentially be excluded from clusters if it falls far from the cluster centers. As described for *k*-means clustering, the procedure was repeated from 1 to *n* clusters and the mean silhouette value was determined. The number of clusters was chosen in a similar manner, where the number of clusters that corresponds with lowest local maximum in mean silhouette values was selected. Using the membership criterion established by Dekkers et al. (2014) (in their analysis of magnetic properties using fuzzy

c-means clustering), directions were excluded from cluster Fisher means if the second highest membership value is greater than 60% of the highest membership value.

Gaussian mixture model (GMM) clustering assumes the data set is a combination of normally distributed data with separate mean values. As in the above methods, clustering was performed incrementally from 1 to *n* clusters, and for each iteration the mean cluster directions and covariances are determined; directions were assigned to the cluster which yielded the greatest posterior probability. For each iteration, the Akaike’s information criterion (AIC), which describes the quality of the model, was determined (Ljung, 1999). The lowest local minimum in AIC was used to determine the number of clusters to describe the data. Cluster analyses are compared with the independent contouring analysis; agreement between the clustering and contouring centers is interpreted as the recognition of a significant cluster grouping.

The gridded data was plotted and contoured with Generic Mapping Tools [Version 5.1.1, Wessel et al., 2013], whereas clustering was determined using the statistical toolboxes accompanying Matlab (The MathWorks, 2015). Results from the spherical contouring and clustering analysis are presented in Figs. 4–6 (a presentation of cluster analysis applied to a synthetic dataset is provided in Supplementary Figs. SM4.1–SM4.3).

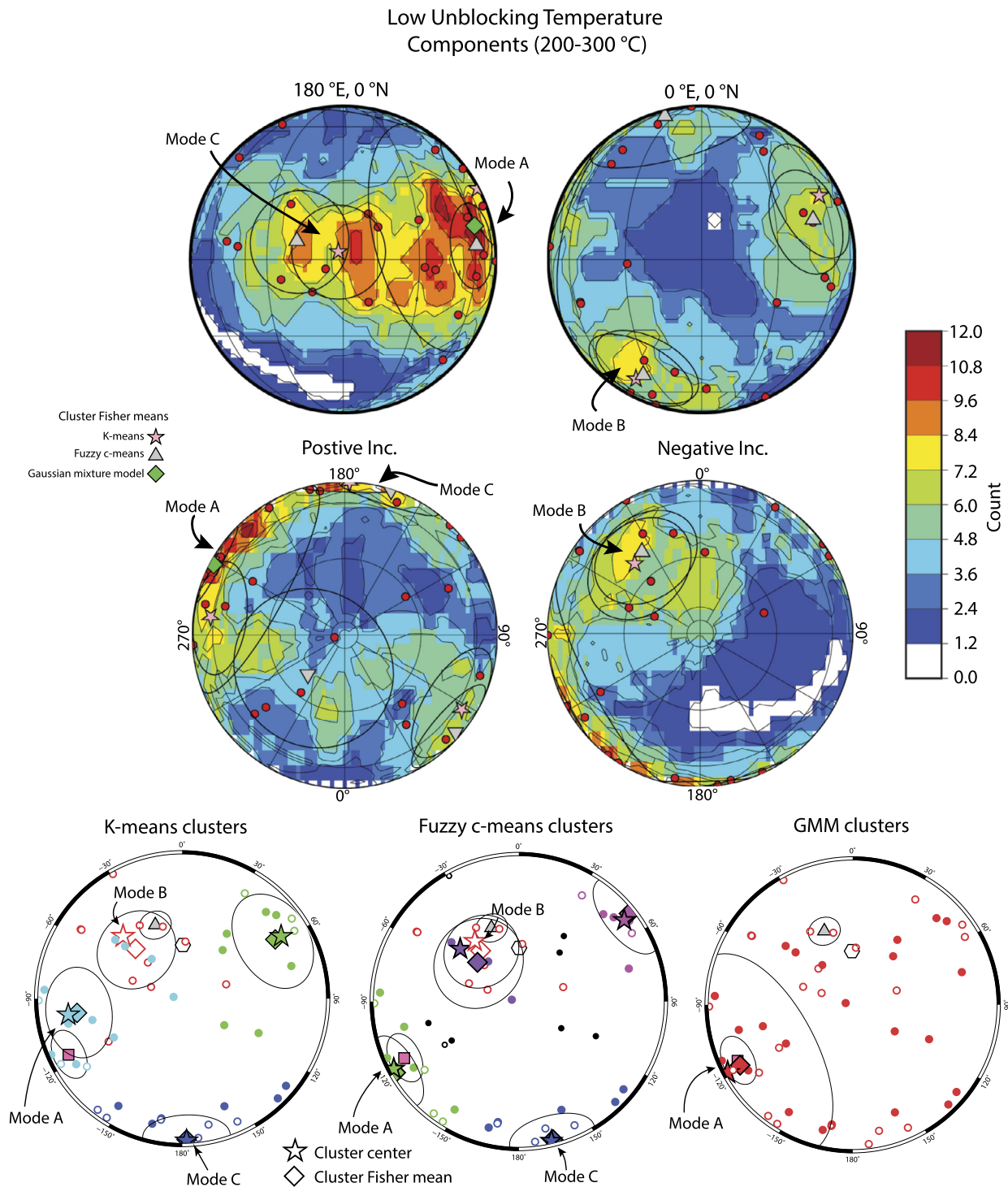


Fig. 4. Spherical contouring and cluster analysis of low unblocking temperature (LT) components. Top row: hemispherical views centered at 0°N showing the results of spherical contouring and cluster analysis. Red points show LT directions. Labels identify cluster modes described in the text. Stars, diamonds and triangles show Fisher means of clustered directions with 95% confidence interval: pink star, k-means clustering; green diamond, Gaussian mixture model clustering; grey triangles, fuzzy c-means clustering. Contour intensity corresponds with density of directions within the counting radius for each grid node. Middle row: polar views of contouring and cluster analyses. Bottom row: equal area stereonets showing the result of clustering analysis applied to LT directions. Colors correspond with grouping assigned during clustering, for fuzzy c-means clustering, black symbols denote directions not assigned to any cluster. Open symbols, negative inclinations; solid symbols, positive inclinations. Stars show cluster centers, diamonds show Fisher mean of directions from each cluster group with α_{95} confidence ellipses. Square: ~2.65 Ga unblocking temperature direction carried by Cr–Fe spinels hosted within fuchsite grains (Cottrell et al., 2016), 95% confidence ellipse shown; triangle, expected direction for ~1 Ga overprint from Warakurna intrusion (Wingate et al., 2002, 2004); hexagon, present field direction for Jack Hills.

5. Results

The k-means clustering approach generally shows a better agreement with contouring analyses; therefore it is our preferred

method of classifying modes in the data. We start by assigning 20% of the data as a threshold for recognition of a data subset using the k-means approach. Fuzzy c-means clustering produced similar cluster mean directions to k-means clustering; using the member-

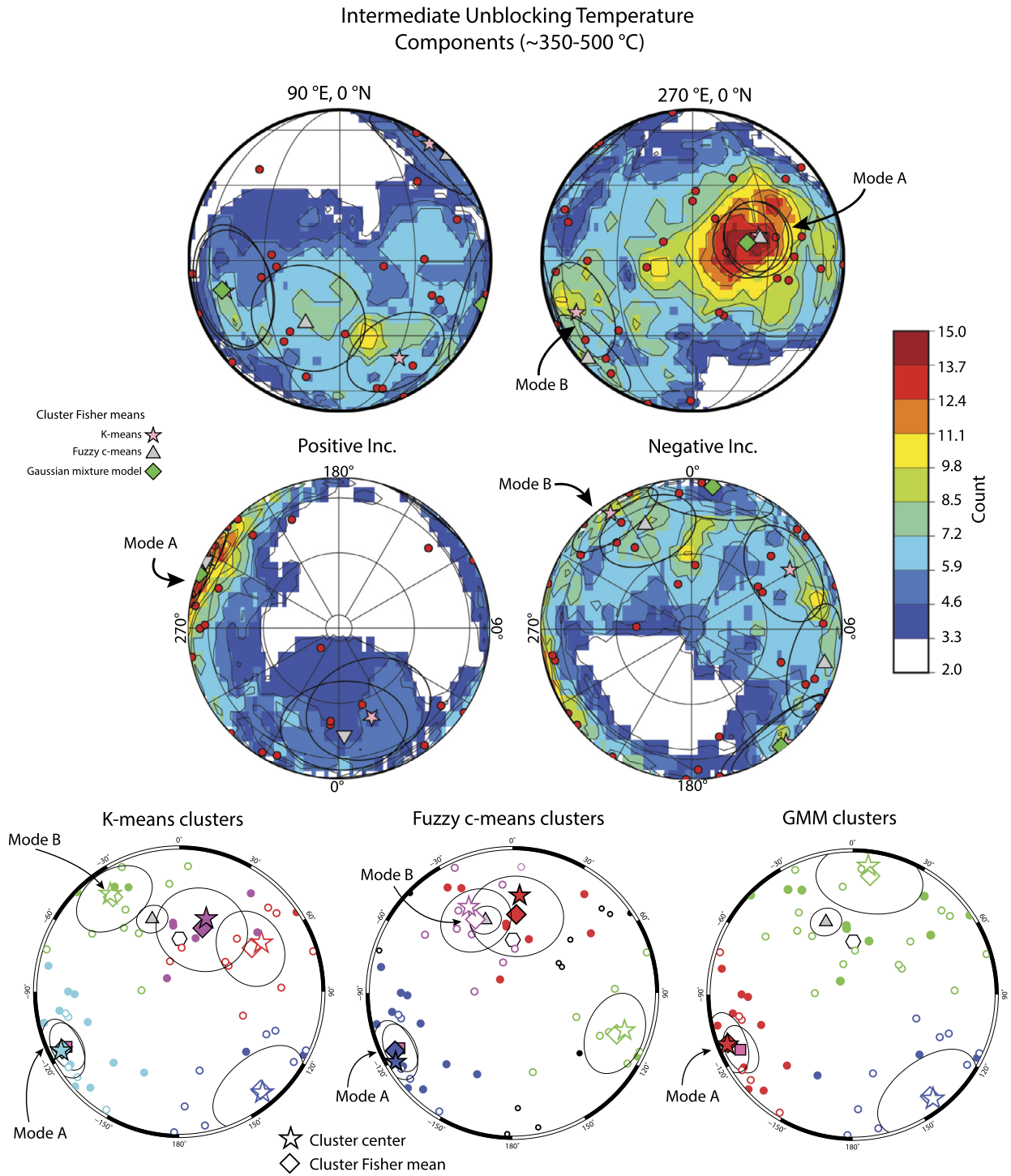


Fig. 5. Spherical contouring and cluster analysis of intermediate unblocking temperature (IT) components. Top row: hemispherical views centered at 0°N showing the results of spherical contouring and cluster analysis. Red points show IT directions. Labels identify cluster modes described in the text. Stars, diamonds and triangles show Fisher means of clustered directions with 95% confidence interval: pink star, k-means clustering; green diamond, Gaussian mixture model clustering; grey triangles, fuzzy c-means clustering. Contour intensity corresponds with density of directions within the counting radius for each grid node. Middle row: polar views of contouring and cluster analyses. Bottom row: equal area stereonets showing the result of clustering analysis applied to IT directions. Colors correspond with grouping assigned during clustering, for fuzzy c-means clustering, black symbols denote directions not assigned to any cluster. Open symbols, negative inclinations; solid symbols, positive inclinations. Stars show cluster centers, diamonds show Fisher mean of directions from each cluster group with α_{95} confidence ellipses. Square: ~2.65 Ga unblocking temperature direction carried by Cr-Fe spinels hosted within fuchsite grains (Cottrell et al., 2016), 95% confidence ellipse shown; triangle, expected direction for ~1 Ga overprint from Warakurna intrusion (Wingate et al., 2002, 2004); hexagon, present field direction for Jack Hills.

ship criterion of Dekkers et al. (2014) directions not belonging to any clusters were identified, generally reducing the number of directions assigned to clusters by ~20% (LT: 8 of 46 directions, 17.4%; IT: 12 of 55, 22%; HT: 11 of 54, 20.4%).

5.1. Identified LT and IT modes

Analysis of the low unblocking temperature range yields 3 modes shared in the contouring and clustering analysis: A, Dec. = 262.3°, Inc. = 27.5°, α_{95} = 21.9°, n = 13 of 46 (k-means clus-

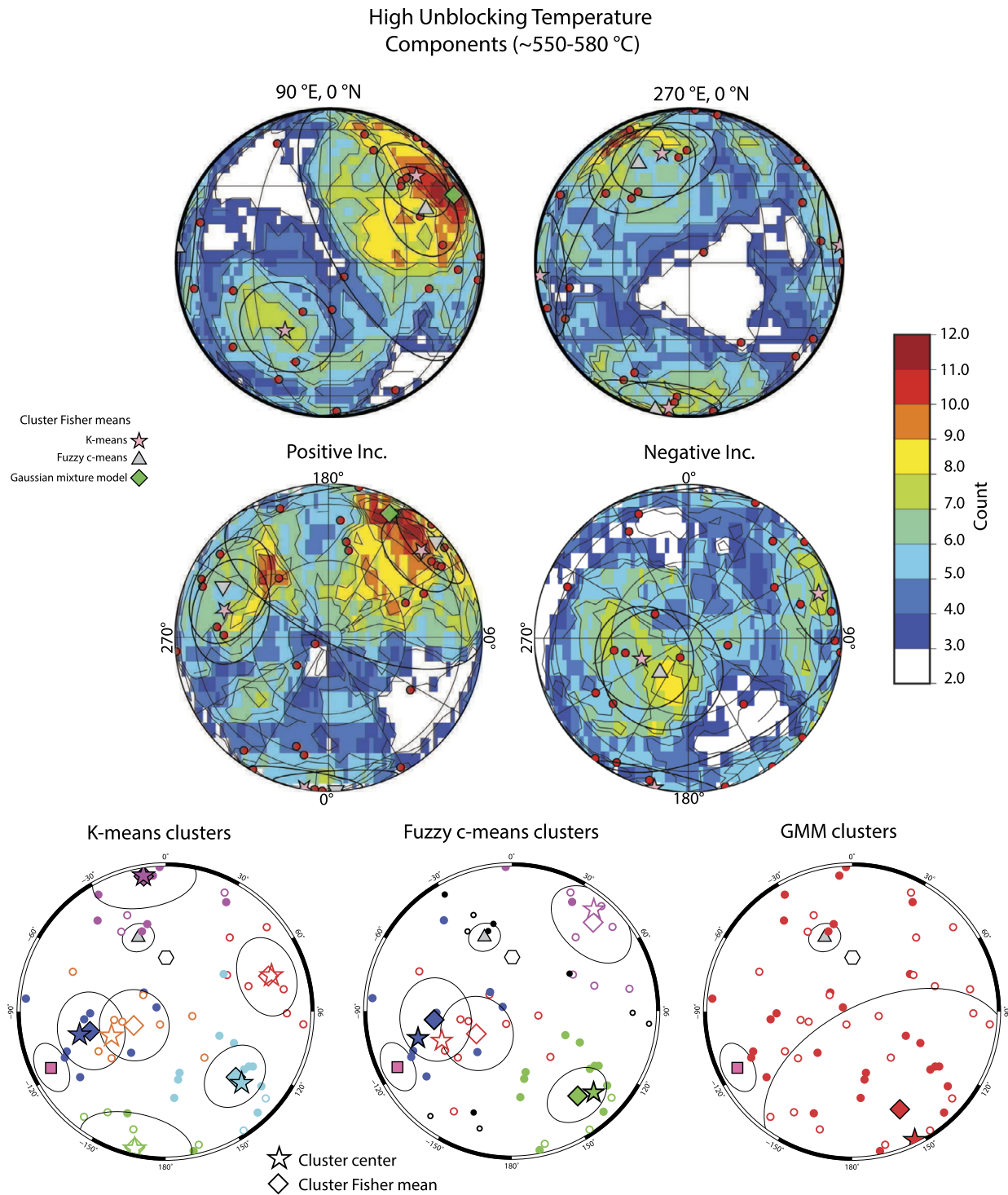


Fig. 6. Spherical contouring and cluster analysis of high unblocking temperature (HT) components. Top row: hemispherical views centered at 0°N showing the results of spherical contouring and cluster analysis. Red points show HT directions. Stars, diamonds and triangles show Fisher means of clustered directions with 95% confidence interval; pink star, k-means clustering; green diamond, Gaussian mixture model clustering; grey triangles, fuzzy c-means clustering. Contour intensity corresponds with density of directions within the counting radius for each grid node. Middle row: polar views of contouring and cluster analyses. Bottom row: equal area stereonets showing the result of clustering analysis applied to HT directions. Colors correspond with grouping assigned during clustering, for fuzzy c-means clustering, black symbols denote directions not assigned to any cluster. Open symbols, negative inclinations; solid symbols, positive inclinations. Stars show cluster centers, diamonds show Fisher mean of directions from each cluster group with α_{95} confidence ellipses. Square: ~2.65 Ga unblocking temperature direction carried by Cr-Fe spinels hosted within fuchsite grains (Cottrell et al., 2016), 95% confidence ellipse shown; triangle, expected direction for ~1 Ga overprint from Warakurna intrusion (Wingate et al., 2002, 2004); hexagon, present field direction for Jack Hills.

tering), 28% of LT components; B, Dec. = 316.8°, Inc. = -51.1°, α_{95} = 22.0°, n = 11 of 46 (k-means clustering), 24% of LT components; and C, Dec. = 178.2°, Inc. = 2.9°, α_{95} = 17.9°, n = 12 of 46 (k-means clustering), 26% of LT components (Fig. 4; Sup-

plementary Figs. SM4.4–SM4.5 and Tables SM4.1–SM4.4). Analysis of the intermediate unblocking temperature range yields 2 similar modes: A, Dec. = 243.8°, Inc. = 9.5°, α_{95} = 13.7°, n = 16 of 55 (k-means clustering), 29% of IT components; B, Dec. = 325.0°,

Inc. = -20.2° , $\alpha_{95} = 19.6^\circ$, $n = 12$ of 55 (k-means clustering), 22% of IT components (Fig. 5; Supplementary Figs. SM4.6–SM4.7 and Tables SM4.5–SM4.10). Directions discussed in this section, unless noted otherwise, are in geographic (*in situ*) coordinates.

When the low and intermediate unblocking temperature ranges are compared, interesting patterns are seen. Mode A is better grouped at intermediate unblocking temperatures relative ($\alpha_{95} = 13.7^\circ$) to low unblocking temperature components ($\alpha_{95} = 21.9^\circ$), suggesting that the latter may be more contaminated by other magnetizations. Therefore, we interpret the intermediate unblocking temperature values from mode A to be the best record of the magnetization. An opposite pattern is seen for the mode B magnetization: the direction is better grouped at low versus intermediate unblocking temperatures.

When using counting circle radii smaller than $\sim 36^\circ$ for contour analysis, the cluster modes discussed above at LT and IT temperatures are present but not well-defined. With a $\sim 16^\circ$ counting radius, at low unblocking temperatures the mode B direction is apparent and there are hints of the mode A cluster direction. For IT directions, with a $\sim 16^\circ$ counting radius the mode A direction is apparent but the mode B direction is less clear.

5.2. Potential LT and IT artifacts

At low unblocking temperatures (~ 200 – 300°C), one cluster method (fuzzy c-means) produced a cluster direction centered in the northwest with a steep, positive inclination that is nominally similar to a 1 Ga overprint (Fig. 4 and Supplementary Tables SM4.3–SM4.4). However, this direction is poorly defined and uses only 4 of the 46 directions ($\sim 9\%$ of LT directions) included in the low unblocking temperature data; one of these directions is in the southeast quadrant. This direction is not recognized in the k-means analysis nor is it seen in the contour analysis for LT data. The direction is also not observed at higher temperatures relevant to the preservation of magnetization carried by magnetite. We suggest that this direction is an artifact of the clustering approach and not a significant direction preserved in the data.

At intermediate temperatures, a cluster with large scatter is identified in the northeast quadrant with positive inclinations (Fig. 3). This cluster is also defined by a small number of directions [6 (k-means approach) or 8 (fuzzy c-means) out of 55, 11% or $\sim 15\%$ of the IT directions, respectively] and has large scatter ($\alpha_{95} = \sim 25^\circ$). This suggests that the identified direction is also an artifact of the clustering approach, and that northeast, positive directions are not a dominant mode of preserved directions in the magnetic record. We also fail to recognize northeast, positive clusters in the cobble conglomerate paleomagnetic data of Weiss et al. (2015), discussed below.

Another possible source for artifacts in these analyses are multicomponent directions. In complexly magnetized rocks, the presence of overlapping unblocking temperature components could have the appearance of a distinct direction that is in fact multicomponent in origin. This may explain the occurrence of the Mode C direction in the LT unblocking components; there is no obvious source for overprinting which would produce that direction; instead it may record mixed components of magnetization.

5.3. Analyses of HT components

Cluster analyses produce only poorly-defined directions within subsets of the HT directions with the exception of one direction [Dec. = 133.0° , Inc. = 34.4° , $\alpha_{95} = 21.9^\circ$, $n = 13$ of 54 (k-means clustering)] comprising 24% of the directions which we call Mode D (Fig. 6 and Supplementary Table SM4.12). We note that in particular the directions of this mode are streaked, with declinations ranging from 57.2° to 146.7° . Contouring analysis for

HT unblocking components yields results far from individual directions, with the exception of a peak near Mode D; all other peaks appear to be artifacts of the large counting radius used (Supplementary Figs. SM4.9 and SM4.10). In fact, contouring analysis using a smaller counting radius ($\sim 16^\circ$) produces no clear evidence for well-defined groups of directions, casting some doubt on the significance of Mode D.

There are hints in directions defined at lower temperatures that Mode D may be an artifact of overprints that are bleeding through to higher unblocking temperatures. Specifically, Mode C of this study, or the component defined at intermediate temperatures of Tarduno and Cottrell (2013), may be contaminating some of the highest unblocking temperature data, resulting in Mode D (Supplementary Fig. SM4.11). This possibility is supported by the range of magnetite grain sizes in Jack Hills cobbles, which include multidomain grains (Dare et al., 2016). One would expect that overprints carried by these larger grains would contaminate magnetizations up to the Curie temperature of magnetite (i.e., $\sim 580^\circ\text{C}$). Overall, these considerations suggest Mode D is a multicomponent magnetization mimicking as a distinct direction. Importantly, if it were a distinct overprint direction of geologic importance, it would be expected to be observed more clearly at lower unblocking temperatures.

5.4. Testing robustness with bootstrap resampling

To assess the robustness of the clustering analysis, a non-parametric, bootstrap approach was used (Efron and Tibshirani, 1986, 1993). A synthetic data set was constructed by randomly drawing n directions from the observed directions, where n is equal in size to the set of observed directions. If a direction was drawn more than once, it was randomly perturbed by $\pm 2.5^\circ$ to allow for multiple draws of the same direction to be weighted appropriately during contouring. Each synthetic data set was clustered using the above methods; this procedure is repeated 100 times to develop a data set of cluster centers from the synthetic data sets.

The resulting data set of cluster centers was divided into clusters using the methods and the Fisher mean direction (and accompanying α_{95} confidence interval) for each group of cluster centers was determined as described above. For the most dominant modes, there is good agreement between observed dataset and the bootstrapped analysis (Fig. 7), suggesting that the clusters determined are robust observations about the distribution of the underlying data.

6. Discussion

Paleointensity data from zircons of the Jack Hills suggest the presence of a geodynamo at 4.2 Ga Tarduno et al. (2015), extending the previously reported 3.4–3.45 Ga data (Tarduno et al., 2010) back in time by more than 700 million years. Diligence must be exercised in selecting zircons for paleomagnetic and rock magnetic analysis to avoid those compromised by alteration. For example, use of large magnetic fields typical of Franz magnetic separators should yield a population of magnetically compromised zircons (cf. Glenn et al., 2017, Supplementary Materials SM1). In contrast, the data reported in Tarduno et al. (2015) come from a highly select set of zircons, chosen from a starting set of some 2500 zircons separated by hand from Jack Hills samples of the Discovery Site.

There are two types of magnetic resetting that must be addressed in the study of Jack Hills zircons. One concerns resetting after zircon formation and prior to emplacements in the conglomerate. Although recognizing that Jack Hills zircons may have

Bootstrap resampling of k-means cluster centers with Fisher mean of each cluster

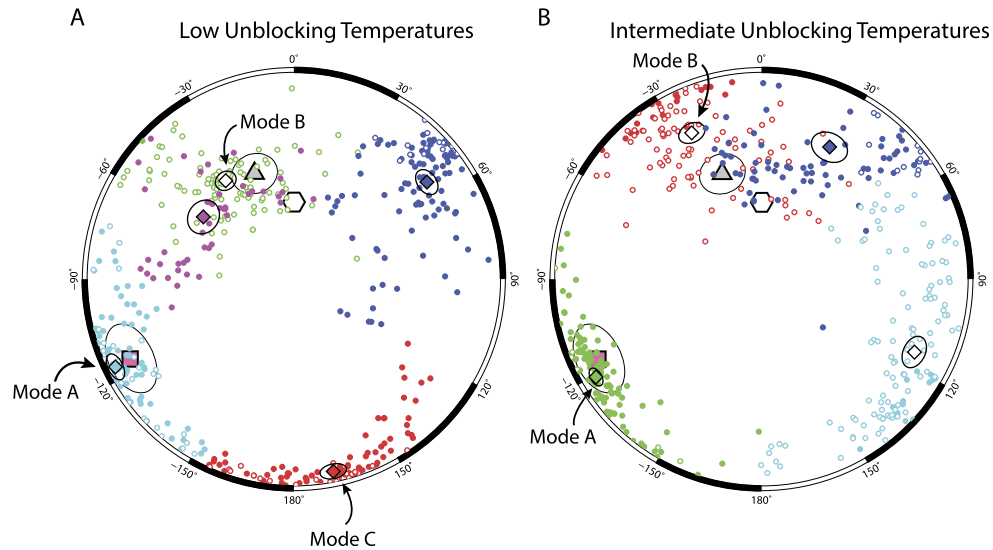


Fig. 7. Non-parametric bootstrap resampling results. Directional data set was resampled 100 times with clustering analysis applied to each synthetic data set. The resulting cluster centers for the 100 resampled data sets were then grouped using k-means clustering. Cluster centers assigned to each group were averaged following Fisher (1953). A) Equal area stereonet showing k-means clustering centers for low unblocking temperature (LT) components. Open symbols, negative inclinations; solid symbols, positive inclinations. Colors show cluster grouping assignment. Diamonds: Fisher mean direction with α_{95} confidence ellipses for each cluster. Labels mark cluster modes described in the text. Square: ~ 2.65 Ga unblocking temperature direction carried by Cr–Fe spinels hosted within fuchsite grains (Cottrell et al., 2016), 95% confidence ellipse shown; triangle, expected direction for ~ 1 Ga overprint from Warakurna intrusion (Wingate et al., 2002, 2004); hexagon, present field direction for Jack Hills. B) Resampling analysis of intermediate unblocking temperature directions using k-means clustering analysis, following (A).

escaped reheating, Tang et al. (2017) have questioned the uniqueness of the Li diffusion interpretation of Trail et al. (2016) that posits the presence of Jack Hills zircons that have not been heated above amphibolite grade metamorphism since formation. Tarduno et al. (2015) carefully examined Pb–Pb data and compared these with data conducted using the same instrument, thereby excluding measurement bias (cf. Harrison et al., 2017, Supplementary Materials SM1). The lack of non-systematic Pb variations typical of reheated zircons, as well as the lack of Pb loss corresponding to hypothetical resetting ages, strongly supports the interpretation that the select zircons studied by Tarduno et al. (2015) are pristine recorders of the Hadean–Eoarchean geomagnetic field.

The second type of resetting concerns that which might occur after conglomerate formation. The first indication that some Jack Hills conglomerate samples are not completely remagnetized came from the studies of cobbles by Tarduno and Cottrell (2013). The salient observations of that study, namely the presence of magnetite and high unblocking temperatures, have now been reproduced by several labs, albeit with differences in resolution that are discussed in depth by Dare et al. (2016). Here, we have considered in more depth the remagnetization history recorded by the Jack Hills cobbles.

We start by reviewing the mode directions. Mode B directions, which are most strongly observed in the lowest unblocking temperature components isolated between ~ 200 – 300 °C, are likely dominated by the present day field (International Geomagnetic Reference Field value for the Jack Hills, Dec. = 0.3° , Inc. = -59.7°). For higher unblocking temperature ranges (~ 350 – 500 °C), the Mode A direction agrees with the magnetic overprint isolated by Cottrell et al. (2016) being carried by secondary Cr–Fe mica fuchsite grains from the Jack Hills Discovery site (Fig. 8A).

A comparison between the Mode A k-means cluster Fisher mean direction from the IT unblocking component after applying a tectonic correction (first uniplunging and then untilting the directions) to restore the bedding to horizontal [using structural data from Spaggiari et al. (2007), bedding plane strike of 244° , dipping

78° N; fold plunge of 12° toward 251°] and ~ 2.65 Ga magnetic overprint carried by fuchsite grains (Cottrell et al., 2016) in stratigraphic coordinates (Dec. = 243.9° , Inc. = 13.2° , $\alpha_{95} = 11.3^\circ$) are indistinguishable at 95% confidence (Fig. 8B). The *in situ* dispersion of an average of the fuchsite direction and the aforementioned Mode A estimate is $k_1 = 21.1$. The post tectonic correction dispersion is $k_2 = 103.6$. The sampling locations of this study and of the Cottrell et al. (2016) study are separated by only ~ 1 – 2 km and therefore likely experienced the same tectonic history. This large improvement in grouping (4.91) is significant at $>80\%$ confidence suggesting that the Mode A direction was acquired after the initial deposition of the conglomerates but prior to (or during) the widespread tectonic folding and plunge, further supporting its ancient age.

Following Cottrell et al. (2016), we interpret the dominant secondary magnetization of the quartzite and the fuchsite characteristic remanent magnetization as ~ 2.65 Ga in age (Rasmussen et al., 2010), coincident with peak metamorphism (as high as ca. 475° C) of the Jack Hills, because these directions are consistent with a well-defined direction from the Yilgarn craton for 2.41 Ga (Smirnov et al., 2013). Differences between the 2.41 Ga reference direction (Smirnov et al., 2013) and the fuchsite and cobble dominant overprint can be explained by modest plate motion, well within the bounds of typical continental plate velocities (1 – 3 cm/yr) [see discussion in Cottrell et al. (2016)]. The highest unblocking temperature components do not support the presence of a directional subset marking a remagnetization of geological significance; the single mode observed seems to be a multicomponent artifact. The lack of evidence for a distinct remagnetization direction is the expected result for data that reflect the preservation of a primary magnetization.

6.1. Remagnetization history

Our model for the remagnetization history at lower temperatures (<500 °C) of the Jack Hills cobble conglomerate units is as follows (Fig. 9): 1) initial deposition of quartzite cobbles bearing

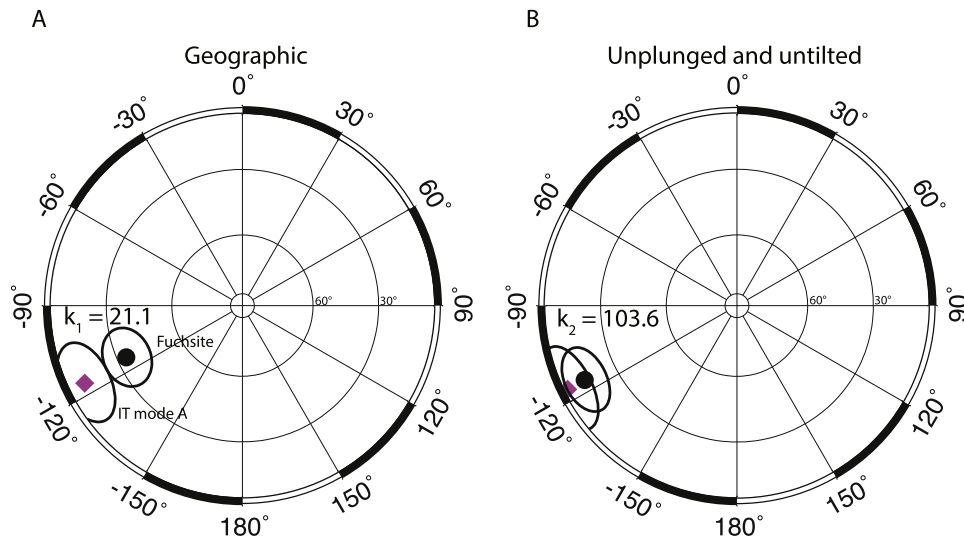


Fig. 8. Comparison of cluster results and fuchsite magnetization. Stratigraphic correction uses structural information from Spaggiari et al. (2007). Equal area stereonet; open symbols, positive inclination; solid symbols, negative inclination. Magenta diamond, mode A intermediate unblocking temperature components k-means cluster with α_{95} confidence ellipse; black circle, fuchsite direction from Cottrell et al. (2016). A. Geographic (*in situ*) coordinates; B. Stratigraphic coordinates. k_1 : dispersion of the Fisher mean (Fisher, 1953) of the IT mode A direction and direction of Cottrell et al. (2016) prior to restoring bedding to horizontal; k_2 : dispersion of the Fisher mean after tectonic correction.

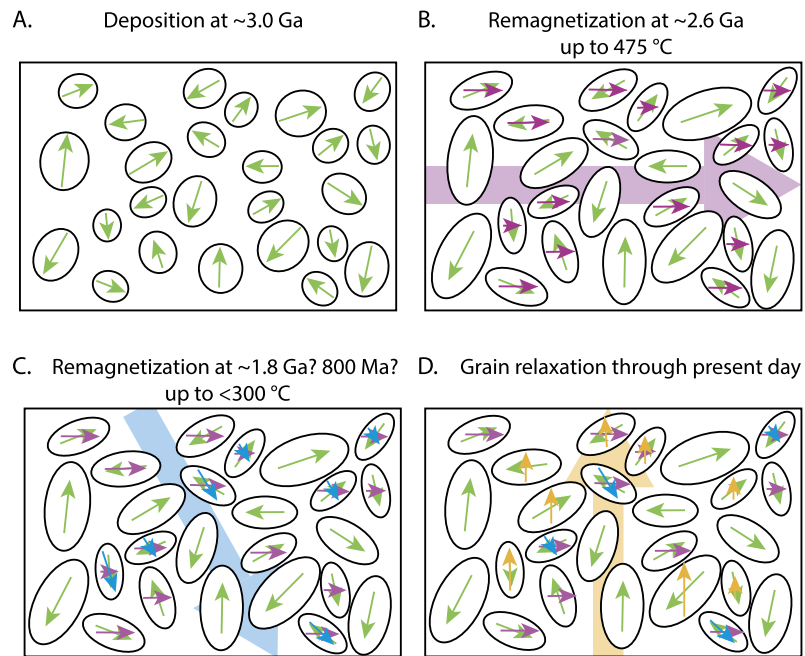


Fig. 9. Acquisition of low unblocking temperature magnetizations in Jack Hills cobbles. A) Initial deposition of cobbles in conglomerate unit, green arrows show primary magnetization directions. Magnetizations are randomly oriented. B) Remagnetization event ~ 2.6 Ga up to 475°C (Rasmussen et al., 2010; Cottrell et al., 2016), resetting magnetizations carried by grains with unblocking temperatures less than $\sim 520^\circ\text{C}$ in a subset of cobbles. Intermediate unblocking temperature components shown with magenta arrows. Large arrow in background denotes geomagnetic field direction. C) Secondary remagnetization event, perhaps at 1.8 Ga and 800 Ma (Rasmussen et al., 2010), at lower temperatures. This imparts a low unblocking temperature magnetization unblocking between 200 and 300°C carried by multidomain grains in a subset of cobbles affected by this event, shown with blue arrows. D) Magnetizations carried by MD grains with low and intermediate unblocking temperatures relax and acquire magnetizations with directions between the present day field and the magnetic field during the initial remagnetization event. Relaxed low and intermediate unblocking temperature directions shown with yellow arrows.

primary detrital magnetizations which unblock at high (approximately $>550^\circ\text{C}$) temperatures, likely at ~ 3.0 Ga. 2) Wide-spread reheating up to $\sim 475^\circ\text{C}$ at ~ 2.6 Ga (Rasmussen et al., 2010; Cottrell et al., 2016), resetting magnetizations carried by grains with unblocking temperatures less than $\sim 520^\circ\text{C}$ [see Dare et al. (2016)] in a subset of cobbles. 3) Subsequent lower temperature (~ 200 to $<300^\circ\text{C}$) reheating, possibly at ~ 1.8 Ga and ~ 800 Ma (Rasmussen et al., 2010), resetting a different, partially overlapping, subset of Jack Hills quartzite cobbles. 4) Magnetizations carried by multidomain

magnetite grains [documented by Dare et al. (2016)] relax, allowing for the acquisition of magnetizations between the initial magnetization (or remagnetization) field direction and the present day field. Finally, modern weathering can enhance the present day field magnetizations in some samples. Differences in low and intermediate unblocking temperature components among Jack Hills quartzite cobbles can reflect variations in the contribution of multidomain magnetic carriers or susceptibility to alteration/weathering of individual cobbles.

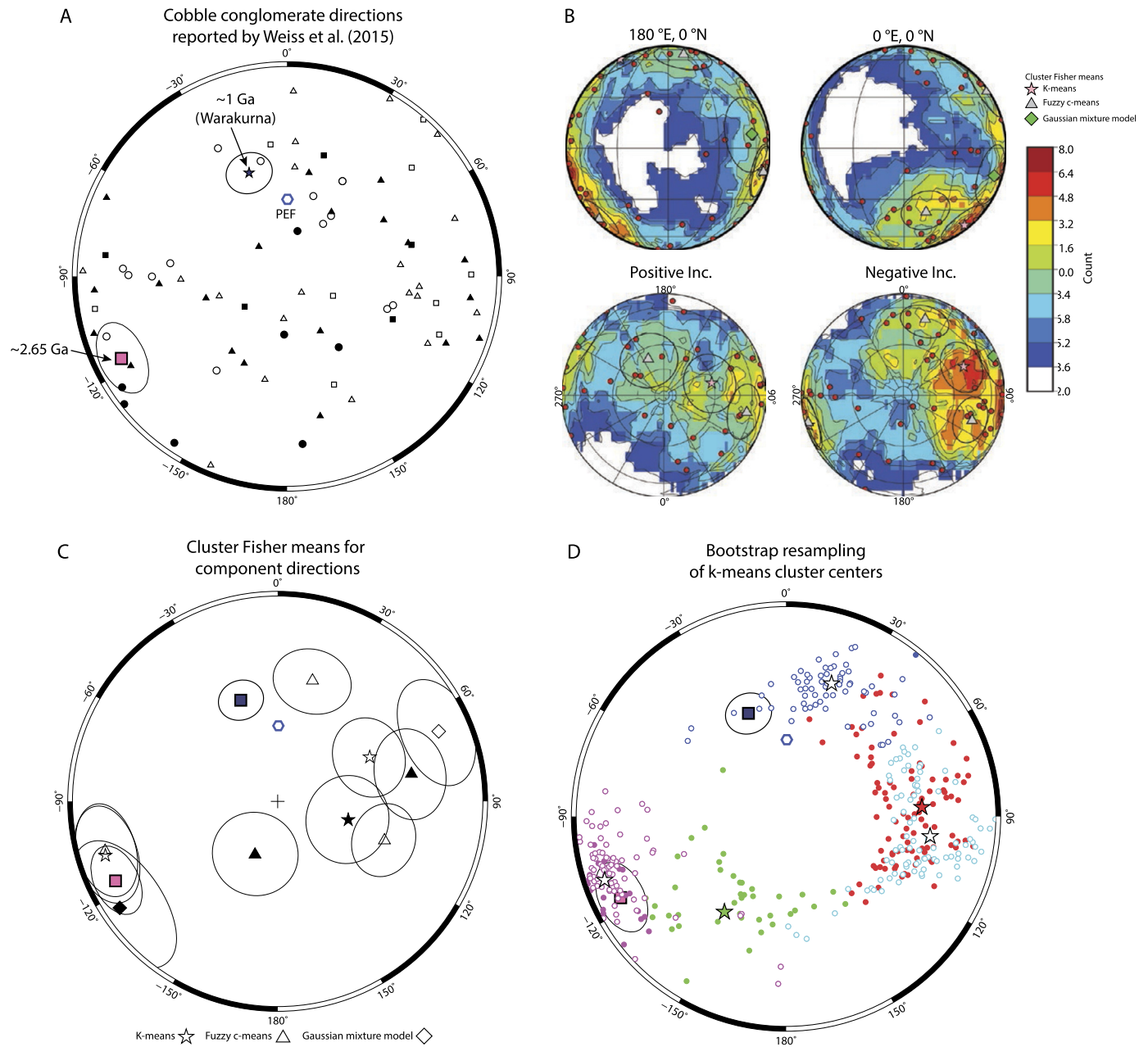


Fig. 10. Spherical contouring and cluster analysis of Jack Hills cobble conglomerate clasts of Weiss et al. (2015). A) Equal area stereonet of showing cobble conglomerate component fits from Weiss et al. (2015). Open symbols, negative inclinations; solid symbols, positive inclinations. Squares, “LT” (nominally low temperature) fits; triangles, “MT” (nominally intermediate temperature) fits; circles, “HT” (nominally high temperature) fits (see text for discussion of component temperature ranges). Blue star: ~1 Ga direction recorded by Warakurna dike (Wingate et al., 2002) with α_{95} confidence ellipse. Blue hexagon: present Earth field (PEF) at the Jack Hills. Magenta square: ~2.65 Ga unblocking temperature direction carried by Cr–Fe spinels hosted within fuchsite grains (Cottrell et al., 2016), 95% confidence ellipse shown. B) Hemispherical and polar views showing the results of spherical contouring and cluster analysis of the entire set of components determined by Weiss et al. (2015) for Jack Hills cobble conglomerate samples. Red points show directions used in spherical contour analysis and clustering. Stars, diamonds and triangles show Fisher mean of clustered directions with 95% confidence interval: pink star, k-means clustering; green diamond, Gaussian mixture model clustering; grey triangles, fuzzy c-means clustering. Contour intensity corresponds with density of directions within the counting radius for each grid node. C) Summary of cluster analysis applied to the entire cobble conglomerate data set of Weiss et al. (2015). Equal area stereonet showing Fisher mean directions with 95% confidence intervals. Open symbols, negative inclination; solid symbols, positive inclination. Star: k-means clustering; triangle: fuzzy c-means clustering; diamond: Gaussian mixture model clustering. Blue square: ~1 Ga direction recorded by Warakurna dike (Wingate et al., 2002) with α_{95} confidence ellipse. Blue hexagon: present Earth field (PEF) at the Jack Hills. Magenta square: ~2.65 Ga unblocking temperature direction carried by Cr–Fe spinels hosted within fuchsite grains (Cottrell et al., 2016), 95% confidence ellipse shown. D) Non-parametric bootstrap resampling results the entire cobble conglomerate data set from Weiss et al. (2015). Directional data set was resampled 100 times with clustering analysis applied to each synthetic data set. The resulting cluster centers for the 100 resampled data sets were then grouped using k-means clustering. Cluster centers assigned to each group were averaged following Fisher (1953). Open symbols, negative inclinations; solid symbols, positive inclinations. Colors show cluster grouping assignment. Diamonds show Fisher mean direction with α_{95} confidence ellipses for each cluster. Blue square: ~1 Ga direction recorded by Warakurna dike (Wingate et al., 2002) with α_{95} confidence ellipse. Blue hexagon: present Earth field (PEF) at the Jack Hills. Magenta square: ~2.65 Ga unblocking temperature direction carried by Cr–Fe spinels hosted within fuchsite grains (Cottrell et al., 2016), 95% confidence ellipse shown.

6.2. Artifactual 1 Ga overprint

Notably, no evidence is found in our data for a pervasive ~1 Ga direction. Our LT and IT data span the limited unblocking tem-

perature range investigated in a separate study by Weiss et al. (2015). Bono et al. (2016) evaluated these claims as they refer to the Discovery outcrop (i.e., the most relevant site to date yielding evidence for a Hadean geodynamo) and found they were based on

an inappropriate use of statistics and a misunderstanding of secular variation. Cottrell et al. (2016) found no evidence for a 1 Ga overprint in secondary minerals of the Jack Hills Discovery outcrop which should have recorded such a hypothetical overprint. Dare et al. (2016) documented the abundant presence of high unblocking temperature magnetite in Jack Hills cobbles as well as inter-laboratory reproducibility of the key high unblocking temperatures. The data of Weiss et al. (2015) also show evidence of high unblocking magnetizations, but these are poorly defined. Dare et al. (2016) also offered guidance on the required experimental procedures.

Weiss et al. (2015) call for a pervasive 1 Ga overprint (i.e., an overprint that is seen everywhere). We have serious concerns with respect to the methods and interpretations of the Weiss et al. (2015) study and their reply (Weiss et al., 2016) to comments pointing out problems with their work (Bono et al., 2016). These include remaining data inconsistencies that indicate unrecognized errors [see Bono et al. (2016), and Supplementary Materials SM1]. Nevertheless, it is illustrative to formally examine their data from cobble-sized metasediments. Because Weiss et al. (2015) propose that the Jack Hills are affected by a pervasive remagnetization, all the Weiss et al. (2015) data can be combined and evaluated together in geographic (*in situ*) coordinates.

Our initial analysis reveals a few intriguing results. Weiss et al. (2015) employ a highly unusual unblocking component assignment scheme, where samples of similar lithologies with nearly identical unblocking temperature components are classified differently [e.g., cobble conglomerate samples D112k.3, 250–325 °C, “LT” (low temperature); D111d.2, 250–325 °C, “MT” (intermediate temperature); D111i.6, 275–325 °C, “HT” (high temperature); D112f.1, 275–325 °C, “HT”]. In this analysis, all unblocking components identified by Weiss et al. (2015) are grouped together for contouring and cluster analysis. There is no evidence in the Weiss et al. (2015) data that a ~1 Ga overprint is preserved in their cobble conglomerate samples over any of the reported magnetic components (Fig. 10; Supplementary Figs. SM4.12–SM4.14). Specifically, the application of our new contouring and clustering approach does not yield any mode which resembles a 1 Ga overprint. However, two clusters are identified using the k-means approach which are consistent with modes A and B from our study (respectively, Dec. = 252.6°, Inc. = −13.1°, α_{95} = 15.5°, n = 21 of 80, ~26%; Dec. = 64.3°, Inc. = −48.9°, α_{95} = 15.0°, n = 32 of 80, 40%). These modes are preserved after the application of the bootstrap resampling analysis.

Thus, at low unblocking temperatures, the data from cobbles from Weiss et al. (2015), Tarduno and Cottrell (2013) and new data reported here are remarkably similar. Differences are that Weiss et al. (2015) interpret these as part of a record of a “pervasive” ~1 Ga remagnetization, a conclusion that their paleomagnetic data from Jack Hills cobbles do not support. This raises the question of whether there is any evidence of a 1 Ga overprint in the Jack Hills sediments; we can find no evidence for this overprint in the sediments of the Discovery site (see Supplementary Materials SM4). We conclude that the interpretation that a 1 Ga overprint affects all Jack Hills lithologies is not supported by the data.

6.3. Age and thermal history of Jack Hills

The age of monazite and xenotime from the Jack Hills near the Discovery site constrains the depositional age of the metasediments to be older than ca. 2.65 Ga and 3.1 Ga respectively (Rasmussen et al., 2010). These constraints, combined with the youngest zircons found in these sediments, has led to the commonly quoted value of ca. 3 Ga as the depositional age near the Discovery Site and for most of the Jack Hills metasediments. However, as noted previously, the identification of much younger zir-

cons, in one case only 50 m from the Discovery Site (Cavosie et al., 2004), forms the basis for the interpretation of tectonic interleaving of younger Proterozoic sediments (Spaggiari, 2007).

This unusual age relationship also exists for the available age data for Jack Hills cobbles. Grange et al. (2010) report results from two cobbles; one contained a single zircon with an age of ca. 1200 Ma and a major peak of ages between 1600 and 1800 Ma. In contrast, another sample contained no zircons younger than 3 Ga; the latter are similar to results from the Discovery Site. Unfortunately, the Grange et al. (2010) samples were collected as float (loose cobbles displaced from their original outcrop) and GPS locations were not recorded. Therefore, the age of the younger sample cannot be related with confidence to the horizons we have sampled for paleomagnetism.

The paleomagnetic analysis discussed here, however, suggests a ~2.65 Ga overprint for select samples, and therefore a depositional age for these samples similar to that of the Discovery outcrop. There is no apparent relation between the sampling location for a given cobble and the clustering of low and intermediate component directions (Supplementary Fig. SM4.8); the key ~2.65 Ga overprint appears to be recorded over the length of the cobbles transect. Therefore, these analyses support an Archean depositional age for at least sediments of this transect and those of the Discovery Outcrop.

7. Conclusions

Sediments of the Jack Hills, because they host the oldest known terrestrial zircons, are of seminal interest for paleomagnetic investigations of the earliest geodynamo. Context for magnetizations held by zircons can be provided by the study of their host rocks. The Jack Hills sediments have been metamorphosed to ~475 °C, and this temperature provides a starting point for understanding the Jack Hills host rock paleomagnetic record: magnetizations isolated at lower temperatures can only tell us about history after deposition (remagnetization), whereas higher unblocking temperature magnetizations can be used to test for the presence/absence of primary magnetizations. Presence of these primary signals would support the veracity of paleomagnetic data from Jack Hills zircons as recorders of the Hadean to Eoarchean geodynamo (Tarduno et al., 2015).

However, the coarse metasediments from the Jack Hills are not ideal magnetic recorders. For example, even on a small scale, pebble conglomerates are internally deformed excluding meaningful field tests. However, as discovered by Tarduno and Cottrell (2013), cobble-sized clasts can contain areas of minimal deformation and recrystallization. Nevertheless, their paleomagnetic record is complex at low unblocking temperatures, likely reflecting nearly 3 billion years of geologic history.

This complexity motivated the development of a new approach. Specifically, cluster analysis on a sphere can be used to identify overprints hidden in complex data sets. Of special note is the apparent failure to reject the hypothesis that directions are drawn from a random distribution in the iconic Watson test whereas cluster analysis and non-parametric tests reveal geologically relevant directional clusters.

In our analysis of a data set of magnetic data from 68 quartzite cobbles, we find no evidence for a 1 Ga direction. We also find no evidence for this event in magnetic data reported from cobbles of Weiss et al. (2015) and therefore we conclude the interpreted pervasive remagnetization at 1 Ga (Weiss et al., 2015) is erroneous (Bono et al., 2016).

Instead, we find evidence for two dominant modes in the cobble data. We interpret the lowest unblocking magnetization to be related to the present day field, perhaps contaminated by viscous magnetizations. The more dominant magnetization matches that

observed from the secondary mineral fuchsite isolated from the Jack Hills (Cottrell et al., 2016); we interpret both as recording the geomagnetic field at ~2.65 billion years ago as observed from the Yilgarn Craton during peak metamorphism of the Jack Hills.

The identification of this secondary magnetization – predicted to be present from peak metamorphic temperatures constrained by geochronological studies – and its difference from the high temperature magnetization held by zircons lends further support for the interpretation that select Jack Hills zircons record a Hadean geodynamo. Preservation of Hadean signals is also supported by the lack of a dominant remagnetization direction in high unblocking temperature data from the quartzite cobbles (the expected result if a primary magnetization component is preserved). Cluster analyses on a sphere holds potential for recovering geologically important magnetic directions hidden in data sets that are complex due to multiple overprints, weak magnetizations and or non-ideal grain mixtures containing unstable particles.

Author contributions

R.K.B. and J.A.T. conducted field studies, M.D., R.D.C. and R.K.B. conducted paleomagnetic measurements. R.K.B. analyzed the data using cluster and non-parametric analyses. G.M. provided structural analysis.

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Appendix A. Supplementary material

Supplementary material related to this article can be found online at <https://doi.org/10.1016/j.epsl.2017.12.007>.

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