Machine Learning-based AFT Annealing Parameter r mr0 from c-axis- projected Reduced Mean Length of Partially Annealed 252 Cf-derived FTs and LA-ICP-MS-derived Chemical Composition Data

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Machine Learning-based AFT Annealing Parameter r_{mr0} from c-axis-projected Reduced Mean Length of Partially Annealed ^{252}Cf-derived FTs and LA-ICP-MS-derived Chemical Composition Data

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Abstract

AFT annealing parameter r_{mr0} relative to apatite standard B2 (Carlson et al., 1999; Ketcham et al., 1999) is re-calibrated here using a combination of natural apatite mixtures from sandstones and selected standards. The standards include well-studied DR, FC, TI, and RN-like (Ca-F-apatite end-member). A machine learning approach is used that predicts r_{mr0} based on independent chemical composition data from LA-ICP-MS.

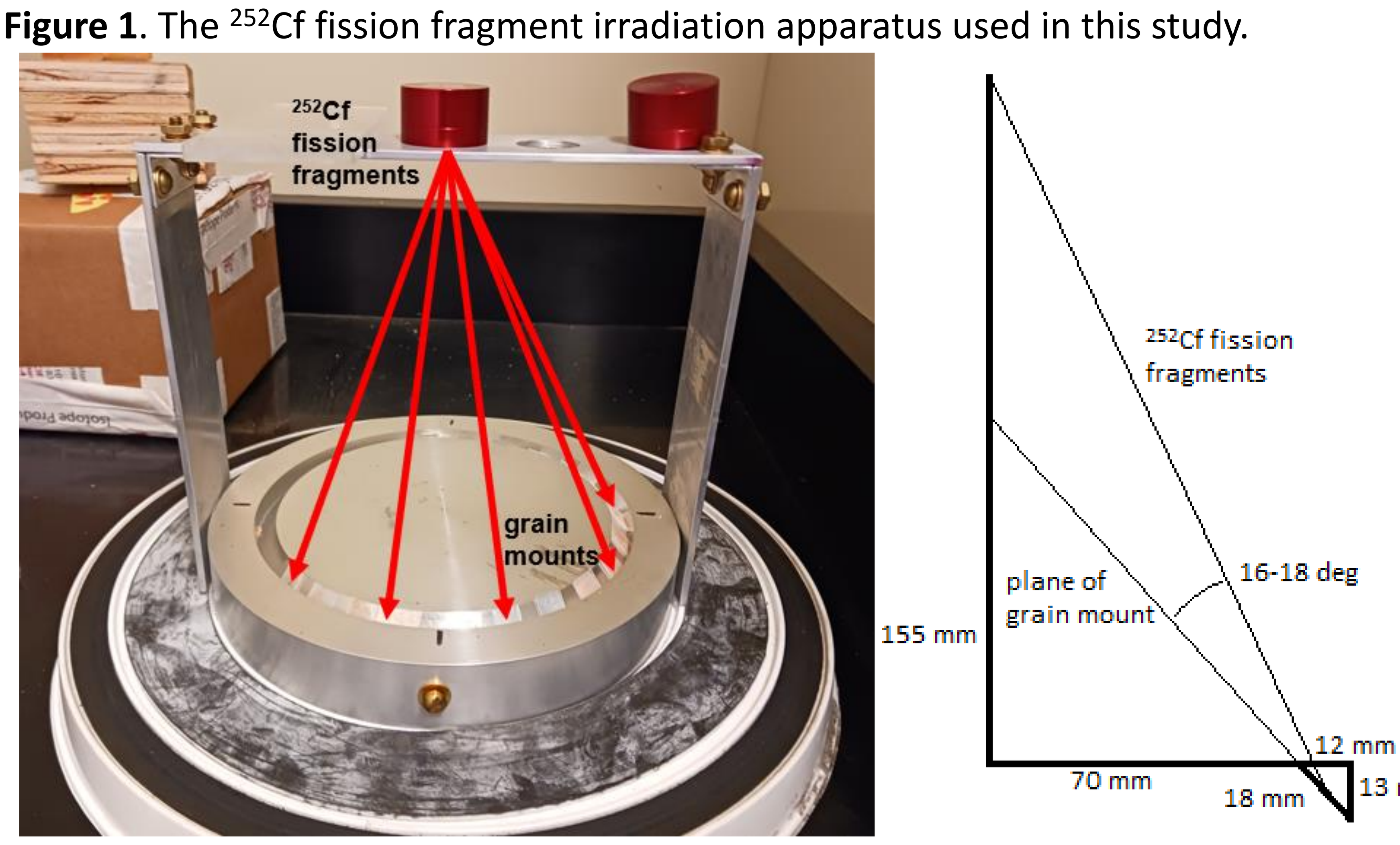
The c-axis-projected (e.g., Donelick et al., 1999), reduced mean length of partially annealed ^{252}Cf-derived FTs is measured and converted to r_{mr0} for each apatite grain studied. Absolute concentrations of Na, Mg, P, S, Cl, Ca, Mn, Fe, As, Sr, Y, 14 REEs, Th, U and relative concentrations of Al, Si, Sc, Br are determined for each grain by LA-ICP-MS using DR and other apatite species as matrix-matched standards (Donelick and Donelick, 2013). Of primary interest to r_{mr0} is: absolute Cl, Mn, Fe, Sr, ΣREEs, and annealing state of natural FTs (pre-annealed or not; t-T path dependence?); of secondary interest is relative Br, absolute Y, Th, U, and Pb-corrected UPb age (t-T path dependence?); of tertiary interest is everything else including the concentrations of individual REEs.

Machine learning regression techniques applied to the data include linear regression, random forests, dense neural networks, and support vector models. We compared the validation results between these regression techniques and examine the importance of each chemical composition feature as determined by the model training. The best performing model identified so far is a random forest regressor, with a 5-fold cross validation mean absolute error of 0.057 +/- 0.004 (1σ) on r_{mr0}.

Table 1. Apatite grains analyzed and ^{252}Cf fission tracks (initial length, annealed 170 h at 295°C) measured per data type for each sample in this study.

Sample	Apatite Description	Grains Initial Condition	Grains Annealed Natural FTs	Grains Unannealed Natural FTs	^{252}Cf Fission Tracks Initial Condition	^{252}Cf Fission Tracks Annealed Natural FTs	^{252}Cf Fission Tracks Unannealed Natural FTs
D3	DR (Carlson et al., 1999)	pending	7	pending	0	407	0
TI	TI (Carlson et al., 1999)	pending	11	pending	0	519	0
FC	FC (Carlson et al., 1999)	pending	pending	pending	0	0	0
MM	RN-like (Carlson et al., 1999)	pending	pending	pending	0	0	0
F5	igneous population - Minn, USA	pending	pending	pending	0	0	0
P10033_031	natural mixture - North Sea	43	--	29	1103	--	236
P10033_032	natural mixture - North Sea	pending	--	12	0	--	105
P10033_033	natural mixture - North Sea	pending	--	14	0	--	92
P10033_035	natural mixture - North Sea	pending	--	68	0	--	274
P10033_036	natural mixture - North Sea	pending	--	49	0	--	80
P10033_037	natural mixture - North Sea	pending	--	58	0	--	209
P10036_003	natural mixture - Utah, USA	pending	143	pending	0	1776	0
P171_001	natural mixture - Utah, USA	pending	168	260	0	1541	2564
P171_003	igneous population - Utah, USA	pending	26	pending	0	1558	0

Figure 1. The ^{252}Cf fission fragment irradiation apparatus used in this study.

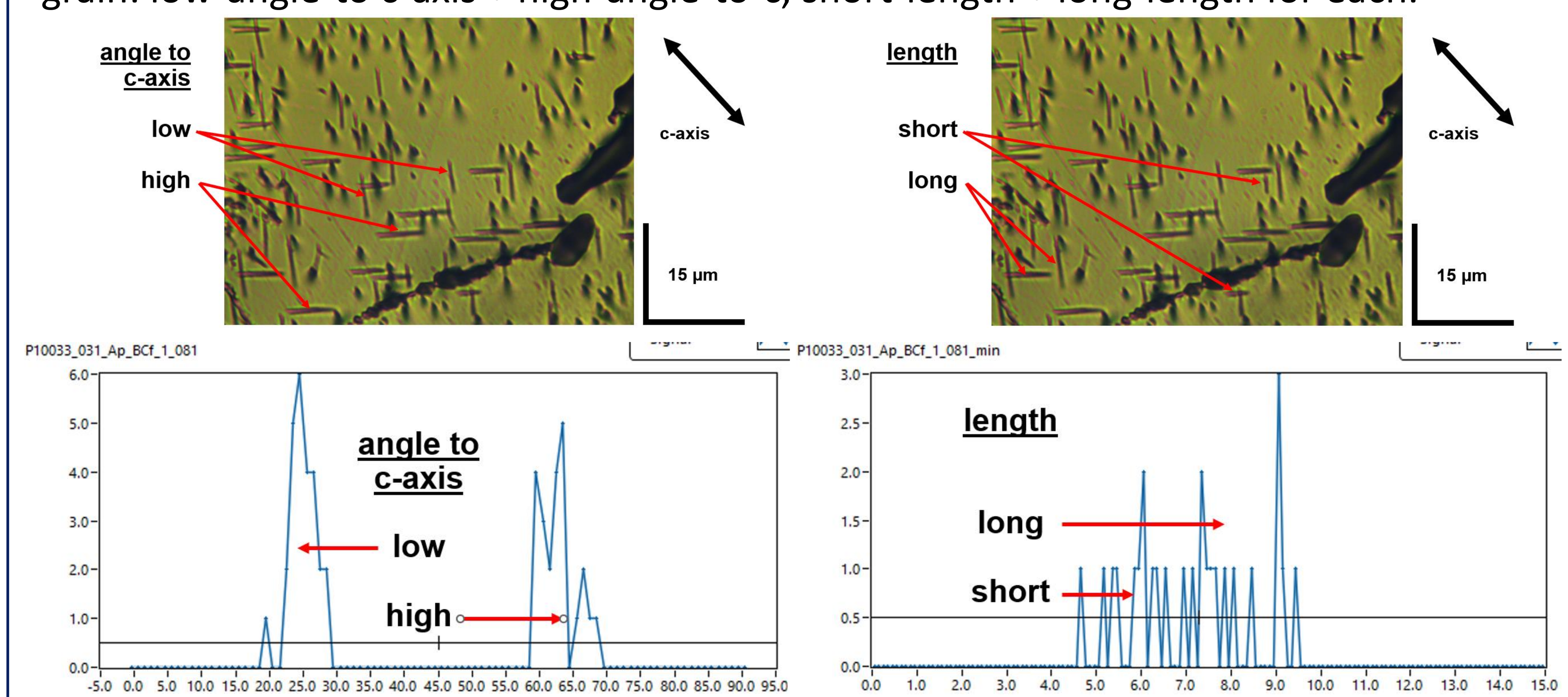


Samples and Methods

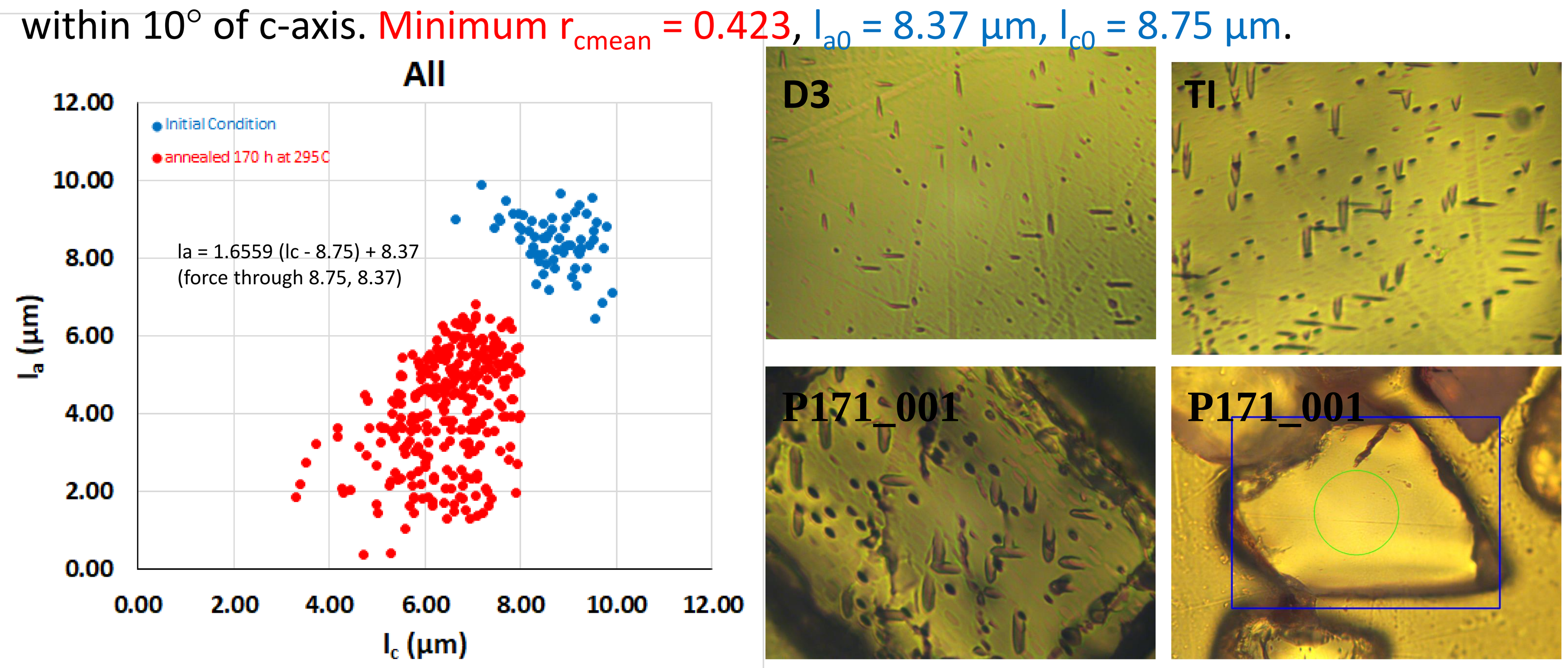
The samples studied are listed in **Table 1**. Apatite grains were mounted in FEP Teflon, polished to a fine finish using 0.3 um Al_2O_3 slurry, and irradiated 24 h in a vacuum (<1 torr) with fission fragment nuclei from an Eckert & Ziegler 50 µCi ^{252}Cf foil (part number CF223010050U; **Figure 1**), rotated 90 degrees, and irradiated an additional 24 h. The ^{252}Cf-derived fission tracks (incident upon and intersecting polished apatite surfaces) were etched using 5.5N HNO_3 for 20 s at 21°C (Donelick et al., 1990). For the *Initial Condition* (**Table 1**), the ^{252}Cf-derived fission tracks were not heated prior to etching. All other ^{252}Cf-derived fission tracks were partially or totally annealed in a muffle furnace for 170 h at 295°C prior to etching. *Annealed* apatite grains (natural fission tracks pre-annealed for 220.5 h at 345°C) and *Unannealed* apatite grains (natural fission tracks untreated) were used (**Table 1**). Data were measured by Ray Donelick using a Nikon E600 microscope, Ludl Kinetec XY-stage, ASI Z-drive, Lumenera Infinity1 digital camera, and Apatite.com Partners' Sample_Scanner.py software. LA-ICP-MS data were collected by Ray Donelick at Washington State University Geoanalytical Laboratory using a NWR UP-213 laser (213 nm, 8 s warmup, 20 s ablation, 20 s washout, 25 µm diameter spot) and Agilent 7700 quadruple mass spectrometer (37 masses for 33 elements). Apatite UPb ages (Chew and Donelick, 2012), and chemical compositions (absolute for Na, Mg, P, S, Cl, Ca, Mn, Fe, As, Sr, Y, 14 REEs, Th, U; relative for Al, Si, Sc, Br; Donelick and Donelick, 2013; Chew et al., 2014) were calculated using Apatite.com Partners' MSData software.

r_{mr0} from ^{252}Cf-derived Fission Track Lengths

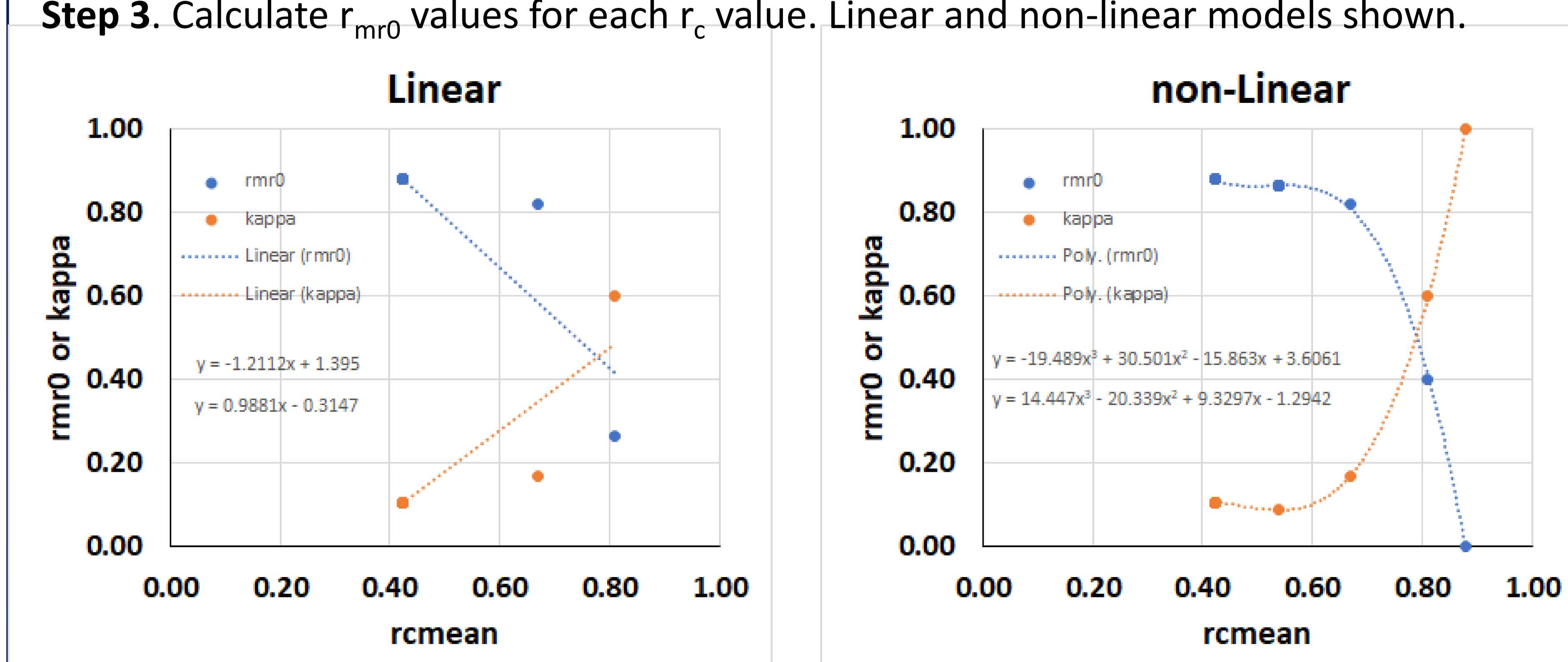
Step 1. Measure mean ^{252}Cf-derived fission track length four populations for each grain: low-angle-to c-axis + high-angle-to-c, short-length + long-length for each.



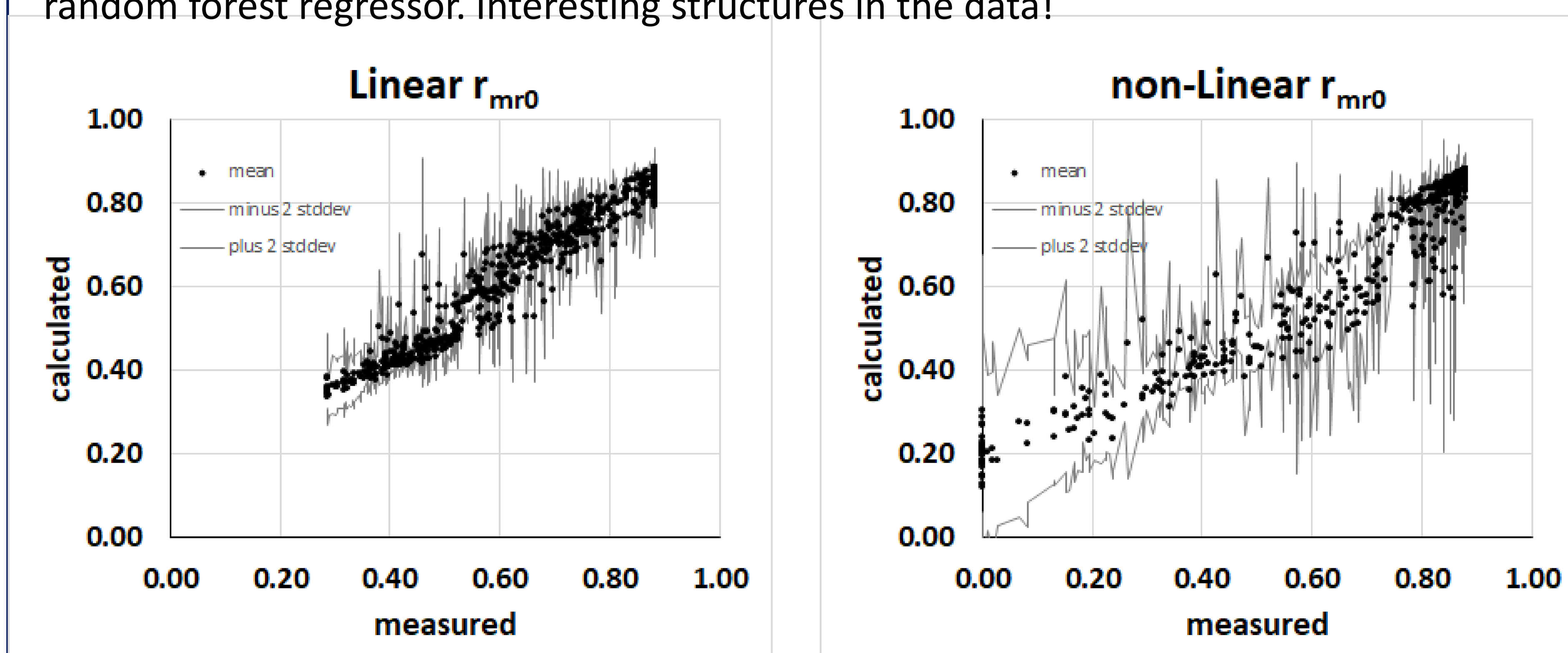
Step 2. Project all low-angle-to-c-axis + long-length mean values onto the c-axis. Totally annealed (bottom right) is measured when ^{252}Cf fission tracks are totally annealed within 10° of c-axis. Minimum r_{cmean} = 0.423, l_{a0} = 8.37 µm, l_{c0} = 8.75 µm.



Step 3. Calculate r_{mr0} values for each r_c value. Linear and non-linear models shown.



Step 4. Apply machine learning regression techniques. Shown here are results for a random forest regressor. Interesting structures in the data!



Acknowledgements

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