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The origin of kimberlitic zircon and the search for a "fingerprint" for superdeep diamonds: enhanced classification of source rock using zircon trace element compositions and machine learning

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Introduction

Zircon occurs in a wide variety of crust- and mantle-derived rocks, including volcanic rocks such as kimberlite, lamproite, MARID (mica-amphibole-rutile-ilmenite-diopside), and more. Some of these volcanic rocks may host diamond and/or sample portions of the earth's uppermost lower mantle. When erupted to the surface, zircon is a relatively useful kimberlite indicator mineral as it is compositionally and physically robust: it can survive weathering in a variety of surface environments (including transport in fluvial or glacial systems). Zircon trace-element compositions are sensitive to the equilibrium mineral assemblage and the original petrogenesis of the source rock (e.g., Hoskin and Ireland 2000).

A previous study applied machine learning (ML) to trace-element compositions of igneous zircons, reported to predict zircon source rock with >75% confidence (e.g., Belousova et al. 2002). Their dataset contained relatively few zircons from kimberlites, carbonatites, and other small degree mantle melts, and did not include zircon from MARID, kamafugite, and other uncommon rock types. Recent studies have applied ML to trace-elements in zircons from a wide range of rock types, using updated statistical approaches (e.g., Zhong et al. 2023; Itano and Sawada 2024). In this study we compile a new database of trace-element compositions for zircons from kimberlite and other igneous rocks such as carbonatites. These zircons include a subset from kimberlites known to contain a population of sub-lithospheric diamonds. Because many of the largest, most valuable diamonds in a given mine are often of sublithospheric origin (Smith et al. 2017), there is considerable interest in "fingerprinting" such diamonds. Zircon from kimberlite is thought to belong to the low-Cr megacryst suite, formed near the base of the lithosphere from asthenosphere-derived melts. As such there may be indirect links between such zircon and superdeep diamonds. Considering recent advances in statistical methods and a greater awareness of the igneous rocks from which zircon may be derived, we use these data to calibrate new ML models for enhanced source rock discrimination, and specifically, the identification of kimberlitic zircon, especially in tropical regions where zircon might be one of the few kimberlite-related minerals to survive the weathering environment.

Dataset and Methods

We have determined the trace-element compositions (REE, Y, Sr, Nb, Ta, Hf, Th, U, and Ti) for >250 new zircons from a wide range of global kimberlites, including the Juína location (Brazil) as well as carbonatites. These data were acquired by LA-ICP-MS at the University of Alberta. We have also compiled >1,500 published trace-element compositions for zircons with known source rocks, including from syenite, nepheline-syenite, ultramafic lamprophyre (UML), kamafugite, MARID, and lamproite (Figure 1). A set of kimberlite zircons were sampled from areas with known superdeep diamond populations, e.g., Juína in Brazil, Monastery in South Africa, and Mothae in Lesotho.

Results and Discussion

Zircons in this study have a wide range of trace-element compositions, though some separation is visible between zircons from many different rock species, for some elements (Figure 1).

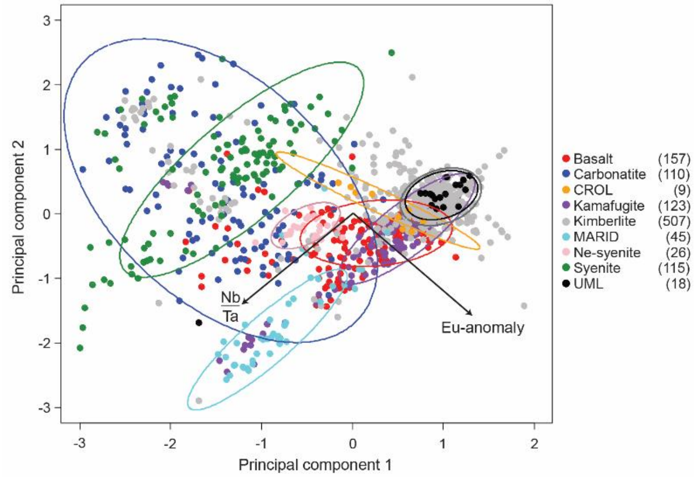

Figure 1: Prinicipal component analysis (PCA) plot for zircon Nb/Ta ratio and Eu-anomalies $(2\times Eu_N)/(Sm_N+Gd_N)$, "$_N$" = chondrite-normalized (McDonough and Sun 1995). Contours correspond to constant Mahalanobis distance with an outlier cutoff equivalent to the 0.95 percentile. CROL = carbonate-rich olivine lamproite, UML = ultramafic lamprophyre.

When the kimberlite zircons compiled in this study are tested using the Classification and Regression Tree (CART) approach of Belousova et al. (2002), ~ 36% misclassify, primarily as carbonatite or syenite. For zircons from MARID and ultramafic lamprophyres – neither types included in the Belousova et al. (2002) study – the former classify as carbonatite, syenite, and kimberlite, and the latter as kimberlite. Recent studies have shown that CART is generally outperformed by other ML methods (Fernández et al. 2014). Hence, new ML approaches applied to larger zircon databases may enhance source rock classification. In this study we calibrate new zircon classification models using the random forest (RF) method (Breiman 2001).

Carbonatites are one of the few rock types where zircon can occur with similar physical dimensions to the megacrysts found in kimberlite. Compositional overlap between the two groups for some elements is evident (Figure 1), and indicated by the classification outcomes produced using the Belousova et al. (2002) approach (above). To improve this, we calibrate RF models for zircon discrimination using Eu-anomalies and Nb/Ta, Th/U, Sm/Nd, and Lu/Gd ratios. Using these variables in our preliminary models we achieve classification error rates of ~ 7±4 % (2σ; 10-fold cross validation). Compositional overlap occurs, due primarily to ~ 6% of compiled kimberlite megacryst zircons having compositions similar to many carbonatitic zircon (e.g., Figure 1), with elevated Nb/Ta ratios and low Eu-anomalies (<0.5).

MARID are an additional suite of mantle-derived rocks for which zircon can have comparable size to kimberlite megacrysts (Hoare et al. 2021). Hence, we use RF to assess whether trace-element compositions can separate zircons from MARID and kimberlite. We calibrate an RF model using Y, Lu, and Nb/Ta and Th/U ratios, with the MARID group composed only of zircons from Bultfontein, Kampfersdam and the nearby Boshoff road dumps. This model has an error rate of ~ 10±5 % (2σ) and identifies the Nb/Ta ratio as the most important discriminant variable, with MARID zircons tending toward higher values (possibly due to equilibrium with rutile, with $D_{Ta}>D_{Nb}$; Klemme et al. 2005). A much smaller subset of MARID zircon (primarily from Bultfontein) have complete REE data; for this subset, MARID zircon tend to have lower Sm/Nd ratios than kimberlite megacrysts. Whether these features are characteristic of MARID zircon or unique to Bultfontein and/or the Boshoff road dumps requires further study.

Finally, we assess whether zircon megacrysts from kimberlites containing a superdeep diamond population have a unique compositional "fingerprint" compared to those from kimberlites dominated by lithospheric diamonds. We calibrate a RF model for classification of zircon from "superdeep" kimberlites by compiling elemental data for zircon megacrysts from the Juína, Monastery, and Mothae kimberlite pipes, using Eu-anomalies and the Lu/Gd, Sm/Nd, Nb/Ta, and Th/U ratios. Classification error rates using RF are ~ 17±5% (2σ) with the Nb/Ta and Th/U ratios found to be important for classification. However, the range of Nb/Ta and Th/U ratios among zircon from kimberlites containing superdeep diamonds in this study is relatively narrower than, and overlaps with, the range of values reported for zircons from kimberlites dominated by lithospheric diamonds; this narrow compositional range may drive some of the discrimination. This result, while preliminary, provides the impetus for further investigation and will require analysis of more zircons from more localities, as well as additional classification variables.

Conclusions

Using a robust database of zircon trace-element compositions from a variety of igneous rocks, including kimberlite, we produce new ML models that can effectively discriminate kimberlitic zircons from those in other igneous rocks, with the exception of ultramafic lamprophyres, generally with error rates <15%. Successful identification of zircon from kimberlites containing superdeep diamonds, however, is more complex and, despite some promise, requires more data for samples from kimberlites with superdeep diamond populations. Our expanding new database for carbonatitic zircons may also have potential applications in using zircon to search for carbonatite-hosted critical metal deposits. In a kimberlite/diamond context, application of these statistical methods to detrital zircons can reduce the cost of exploration or misdirection of exploration efforts.

References

Belousova EA, Griffin WL, O'Reilly SY, Fisher NI (2002) Igneous zircon: trace element composition as an indicator of source rock type. Contributions to Mineralogy and Petrology 143:602-622

Breiman L (2001) Random forests. Machine Learning 45, pp. 5-32

Fernández-Delgado M, Cernadas E, Barro S, Amorim D (2014) Do we need hundreds of classifiers to solve real world classification problems? Journal of Machine Learning Research 15:3133-3181

Hoare BC, O'Sullivan G, Tomlinson EL (2021) Metasomatism of the Kaapvaal craton during Cretaceous intraplate magmatism revealed by combined zircon U-Pb isotope and trace element analysis. Chemical Geology 578:120302

Hoskin P, Ireland T (2000) Rare earth element chemistry of zircon and its use as a provenance indicator. Geology 28:627-630

Itano K, Sawada H (2024) Revisiting the geochemical classification of zircon source rocks using a machine learning approach. Mathematical Geosciences

Klemme S, Prowatke S, Hametner K, Günther D (2005) Partitioning of trace elements between rutile and silicate melts: implications for subduction zones. Geochimica et Cosmochimica Acta 69:2361-2371

McDonough WF, Sun S-s (1995) The composition of the Earth. Chemical Geology 120:223-253

Smith EM, Shirey SB, Wang W (2017) The very deep origin of the world's biggest diamonds. Gems & Gemology 53(4):388-403

Zhong SH, Liu Y, Li SZ, Bindeman IN, Cawood PA, Seltmann R, Niu JH, Guo GH, Liu JQ (2023) A machine learning method for distinguishing detrital zircon provenance. Contributions to Mineralogy and Petrology 178:35