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Plagioclase-saturated hygrothermobarometry and plagioclase-melt equilibria using machine learning

KYRA CUTLER[1], MIKE CASSIDY[2] AND JONATHAN D. BLUNDY[3]

[1]University of Oxford
[2]University of Birmingham
[3]Oxford University
Presenting Author: kyra.cutler@stx.ox.ac.uk

Defining magma crystallisation conditions is critical for understanding how magmatic systems evolve and lead to eruptions. Compositions of single phases and co-existing liquids are often used to determine pre-eruptive temperatures, water contents, and crystallisation depths of magma by applying various thermobarometers and hygrometers. However, despite the numerous hygrothermobarometers available, large uncertainties are still associated with constraining P-T- X_{H2O} estimates, particularly pressure.

Here we use random forest machine learning [1] to test whether we can refine the existing range of plagioclase-based hygrothermobarometers, as well as create a model for predicting equilibrium plagioclase compositions (anorthite, An = [molar Ca/(Ca + Na + K)] appropriate for a broad range of hydrous and anhydrous melt compositions. A calibration dataset of plagioclase-liquid pairs (n=1035) from anhydrous/nominally anhydrous, water-saturated and water-undersaturated experiments was compiled and filtered to ensure equilibrium. Examples of equilibrium filters include incorporating experiments with a quenched liquid fraction >50% and checking if electron microprobe totals are between 97.0–101.5 wt.% (including H_2O). In general, models are calibrated on a range of melt compositions (SiO_2: 37.1–79.9 wt.%; Na_2O + K_2O: 0.3–12.5 wt.%) that crystallised plagioclase (An_{16-100}) at conditions of 0–2000 MPa, 664–1355 °C, and H_2O concentrations up to 11.20 wt.%. We evaluate all models by assessing the variation of root mean square error (RMSE) and coefficient of determination (R^2) values derived from carrying out multiple replications of the workflow [2] (random training/testing set splitting --> 10-fold cross-validation). A notable outcome is that the liquid and plagioclase-liquid models perform as well as each other with similar metrics (median liquid RMSEs: T-independent hygrometer = 1.0 wt.%; T-dependent hygrometer = 0.65 wt.%; H_2O-independent thermometer = 36.5°C; H_2O-dependent thermometer = 24°C; H_2O-dependent barometer = 74 MPa; T and H_2O-independent An content = 6 mol%), highlighting the overall utility of the melt in recovering P-T-X_{H2O}-$Plag_{An}$ conditions. The plagioclase-saturated melt models have been applied to several case studies with the new estimates compared to previous studies.

[1] Simms J et al. (2014) *IEICE TRANS INF & SYST*, DOI: 10.1587/transinf.E97.D.1677

[2] Petrelli M et al. (2020) *JGR: Solid Earth*, DOI: 10.1029/2020JB020130