Refined estimation of Li in mica by a machine learning method

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ABSTRACT

Li-rich micas are crucial in the exploration for and exploitation of Li resources. The determination of Li in mica using classical bulk chemical methods or in situ microanalytical techniques is expensive and time-consuming and has stringent requirements for the quality of micas and reference materials. Although simple linear and nonlinear empirical equations have been proposed, they are inconsistent with the complex physicochemical mechanisms of Li incorporation and commonly lead to large errors. In this study, we introduce a refined method of multivariate polynomial regression using a machine learning algorithm to estimate Li from multiple major oxide abundances. The performance of our regression model is evaluated using the coefficient of determination (R^2) and the root-mean-square error (RMSE) of the independent test sets. The best-performed models show R^2 of 0.95 and a RMSE of 0.35 wt% for the test set of data set 1 (all compiled data, n = 2124) and R^2 of 0.96 and a RMSE of 0.22 wt% for the test set of data set 2 (only data obtained using in situ techniques, n = 1386). Our results indicate that integration of electron probe microanalysis and multivariate polynomial regression (based on data set 1) presents a robust and convenient approach to quantify Li contents in micas. The application of the proposed approach to micas from central Inner Mongolia, NE China, suggests that in addition to the Weilasituo ore bodies, the Jiabusi granite and greisen and the Shihuiyao metamorphic sediment formation have good potential for Li exploration. Our study also provides preliminary constraints on the genesis of Li deposits.

Keywords: Lithium, mica, multivariate polynomial regression, machine learning, Li resources