The Numerical Optimization of Isotope Dilution Analysis

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In the past years, isotope dilution analysis (IDA) has been widely applied in the highly accurate and precise determination of elemental concentrations in geological and environmental samples.With the development of the new mass spectrometry technique, IDA has been extended to study elemental speciation, low concentration samples (~ppt) and the elemental absolute concentration calibration of geological and environmental reference materials[1-3].

Currently, the key factors restricting the IDA applications are difficult to accurately control the optimal proportion of the single spike in the spike-sample mix, especially for the determination of low concentration samples. In order to solve this problem, we took ^{84}Sr spike as an example, and first introduced the Monte – Carlo method to simulate the optimal value of the ratio between the sample and the ^{84}Sr spike. The simulated results shows that the optimum spike (^{84}Sr) to sample (^{88}Sr) ranges from 0.05 to 8, and the optimal ratio($^{84}Sr_{spk}$ / $^{88}Sr_{spl}$) is approximate 1. In addition, we did some evaluations for the IDA numerical optimization results at different isotopic purity of ^{84}Sr spike and differently extracted isotopic ratios. The result displays that: 1. with increasing the purity of the isotope, the optimal ratios of spike to sample rises to higher values and the relative uncertainty at the optimum exhibits a samller value; 2. if we extracted the ratios of ^{88}Sr and ^{84}Sr, the accuracy and precision of the obtained concentration is the highest, and $^{86}Sr/^{84}Sr$ is the second, $^{87}Sr/^{84}Sr$ is the lowest.

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