Application Note: 30111

Interference Corrections in Isotope Ratio Measurements Using MC-ICP-MS: Examples for Nd-Sm

Key Words

- **NEPTUNE**
- **Interference Correction**
- **Multicollector ICP-MS**
- **Neodymium**
- **Samarium**

Introduction

Isobaric interferences are one of the major limitations on the accuracy of isotope ratio measurements made by MC-ICP-MS, and thus, accurate interference corrections are required to achieve precise and accurate isotope ratio measurements. One of the main difficulties in performing interference corrections is how to accurately and precisely assess the mass bias of the interfering isotope(s). We describe and compare the results from three strategies for performing interference corrections, using Nd-Sm data measured on the Thermo Scientific NEPTUNE MC-ICP-MS.

Strategies for Interference Corrections

Neodymium suffers from isobaric interferences from samarium on masses 144, 148 and 150. If the Sm isotope composition of the sample is known, the measurement of the abundance of one interference-free Sm isotope, i.e., ^{147}Sm or ^{149}Sm, allows the calculation of the abundances of the other (interfering) Sm isotopes, i.e., ^{144}Sm, ^{148}Sm and ^{150}Sm. Normally, the IUPAC (International Union of Pure and Applied Chemistry) tabulation of the natural abundances of the isotopes serves as the basis for performing these calculations for interference corrections. If the magnitudes of the interfering isotopes are significant, it becomes necessary to take mass bias into account in order to make an accurate calculation of the abundances of the interfering isotopes. Sm has two isotopes that are interference-free (^{147}Sm and ^{149}Sm). By comparing the measured ^{147}Sm/^{149}Sm ratio with the true ^{147}Sm/^{149}Sm ratio, it is possible to assess the mass bias for Sm. This calculated mass bias factor allows to perform an accurate correction for the interferences of Sm isotopes on Nd. For isotopic systems with just one isotope available for the interference correction, mass bias can be estimated from the isotopes being measured (^{85}Rb in case of Sr).

Here, we consider three cases of interference corrections for Sm:

Method 1: Interference correction without considering mass bias for Sm

The abundances of ^{144}Sm, ^{148}Sm and ^{150}Sm are calculated from the measured intensity of ^{147}Sm and the Sm isotopic abundance data from IUPAC.

Method 2: Interference correction including a mass bias factor for Sm which is based on the measurement of ^{147}Sm/^{149}Sm

The change in relative abundances of Sm isotopes due to mass bias is corrected using the mass bias factor for Sm based on the measured ^{147}Sm/^{149}Sm isotope ratio. The abundances of ^{144}Sm, ^{148}Sm and ^{150}Sm are calculated using the measured intensity of ^{147}Sm and the corrected (mass-bias induced) abundance ratios for Sm.

Method 3: Interference correction considering a mass bias factor for Nd which is based on the measurement of ^{146}Nd/^{144}Nd

The change in relative abundances of Sm isotopes due to mass bias is corrected using the mass bias factor for Sm based on the measured ^{146}Nd/^{144}Nd isotope ratio. The abundances of ^{144}Sm, ^{148}Sm and ^{150}Sm are calculated using the measured intensity of ^{147}Sm and the corrected (mass-bias induced) abundances for Sm. This must be done iteratively, because the normalizing ratio (^{146}Nd/^{144}Nd) also suffers from Sm interference. The initial stage of the correction follows the same procedure described in Method 1, thus without considering mass bias. Based on this interference correction a first estimation of the Nd mass bias is calculated (step 1). This initial estimation of the instrumental mass bias is then taken to calculate the abundances of ^{144}Sm, ^{148}Sm and ^{150}Sm. Based on this second interference correction, the Nd mass bias is calculated again (step 2). These steps are repeated several times until the mass bias correction algorithm converges to a constant Nd mass bias value (compare the values for ^{146}Nd/^{144}Nd in every step in the example given below).

All three types of interference corrections can be performed on-line using the multicollector software that is standard with the NEPTUNE MC-ICP-MS. Here we demonstrate the calculation of the ^{143}Nd/^{144}Nd ratio. This ratio is corrected for the interference of ^{144}Sm according to the three methods described above. The final ratio is then corrected for mass fractionation using ^{146}Nd/^{144}Nd. These measurements were done on a solution of 200 ppb Nd doped with 10 ppb Sm (both from Merck).

Screenshots of the Method Editor program from the multicollector software are included illustrating how these on-line calculations are handled.

Mass bias correction

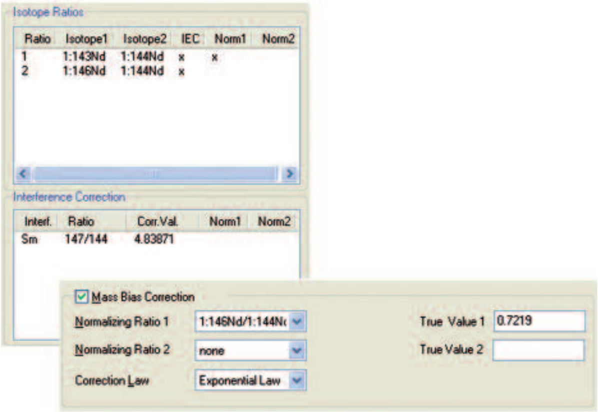
The normalizations are performed according to the exponential law, where X and R are the isotopic ratios of masses m1/m2 and m3/m4, respectively. M refers to the measured isotope ratio, T refers to the true (unfractionated) isotope ratio, and a = ln[mass3/mass4]/ln[mass1/mass2].

$$\frac{X_M}{X_T} = \left[\frac{R_M}{R_T}\right]^a$$

Method 1: Interference correction without considering mass bias for Sm

Variables	Description	Value
abu144	abundance ^{144}Sm in % (IUPAC)	3.1
abu147	abundance ^{147}Sm in % (IUPAC)	15
^{147}Sm/^{144}Sm	abu147/abu144	4.83871
m1	mass ^{146}Nd	145.91311
m2	mass ^{144}Nd	143.91008
m3	mass ^{143}Nd	142.90981
m4	mass ^{144}Nd	143.91008
R_T	true ratio ^{146}Nd/^{144}Nd	0.7219
R_M	measured ratio ^{146}Nd/^{144}Nd	
X_T	true ratio ^{143}Nd/^{144}Nd	
X_M	measured ratio ^{143}Nd/^{144}Nd	
a	ln[m3/m4]/ln[m1/m2]	-0.504603
Measured Data		
$^{143}Nd_M$	measured intensity ^{143}Nd (V)	0.9592
$^{144}(Nd+Sm)_M$	measured intensity ^{144}(Nd+Sm) (V)	1.919
$^{146}Nd_M$	measured intensity ^{146}Nd (V)	1.412
$^{147}Sm_M$	measured intensity ^{147}Sm (V)	0.09056
Calculation of ^{144}Nd corrected for interference of ^{144}Sm		
^{144}Sm	$^{147}Sm_M/(^{147}Sm/^{144}Sm)$	0.01872
^{144}Nd	$^{144}(Nd + Sm)_M - {}^{144}Sm$	1.900
Calculation of ^{143}Nd/^{144}Nd corrected for mass fractionation		
R_M	$^{146}Nd_M/^{144}Nd$	0.742807
X_T	$X_M/([R_M/R_T]$^a)	0.512046

Table 1: Step-by-step calculation of the true ^{143}Nd/^{144}Nd ratio for method 1



Isotope Ratios

Ratio	Isotope1	Isotope2	IEC	Norm1	Norm2
1	1:143Nd	1:144Nd	x	x	
2	1:146Nd	1:144Nd	x		

Interference Correction

Interf.	Ratio	Corr.Val.	Norm1	Norm2
Sm	147/144	4.83871		

☑ Mass Bias Correction

Normalizing Ratio 1: 1:146Nd/1:144N
Normalizing Ratio 2: none
Correction Law: Exponential Law
True Value 1: 0.7219
True Value 2:

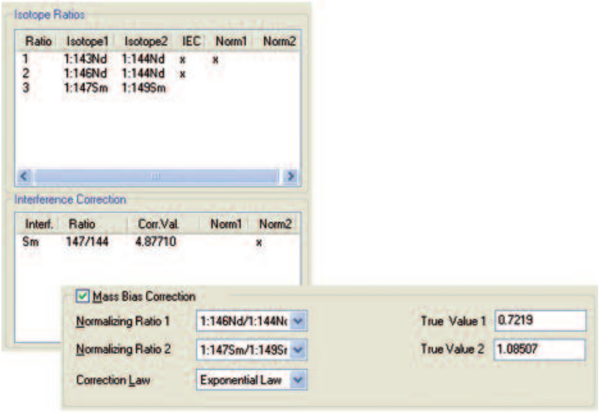
Figure 1: Screenshot of the Method Editor (evaluation pane) for method 1

^{143}Nd/^{144}Nd is interference corrected (IEC) using the ^{147}Sm/^{144}Sm ratio from IUPAC without considering mass bias for Sm. The ^{143}Nd/^{144}Nd ratio is then corrected for mass fractionation using Normalizing Ratio 1 (^{146}Nd/^{144}Nd = 0.7219).

Method 2: Interference correction including a mass bias factor for Sm based on the measurement of ^{147}Sm/^{149}Sm

Variables	Description	Value
m1	mass ^{146}Nd	145.91311
m2	mass ^{144}Nd	143.91008
m3	mass ^{143}Nd	142.90981
m4	mass ^{144}Nd	143.91008
R_T	true ratio ^{146}Nd/^{144}Nd	0.7219
R_M	measured ratio ^{146}Nd/^{144}Nd	
X_T	true ratio ^{143}Nd/^{144}Nd	
X_M	measured ratio ^{143}Nd/^{144}Nd	
a2	ln[m3/m4]/ln[m1/m2]	-0.504603
m5	mass ^{147}Sm	146.91489
m6	mass ^{149}Sm	148.91718
m7	mass ^{147}Sm	146.91489
m8	mass ^{144}Sm	143.91199
$R^{Sm}{}_T$	true ratio ^{147}Sm/^{149}Sm	1.08507
$R^{Sm}{}_M$	measured ratio ^{147}Sm/^{149}Sm	
Y_T	true ratio ^{147}Sm/^{144}Sm	4.87710
Y_M	measured ratio ^{147}Sm/^{144}Sm	
a1	ln[m7/m8]/ln[m5/m6]	-1.52558
Measured Data		
$^{143}Nd_M$	measured intensity ^{143}Nd (V)	0.9592
$^{144}(Nd+Sm)_M$	measured intensity ^{144}(Nd+Sm) (V)	1.919
$^{146}Nd_M$	measured intensity ^{146}Nd (V)	1.412
$^{147}Sm_M$	measured intensity ^{147}Sm (V)	0.09056
$^{149}Sm_M$	measured intensity ^{149}Sm (V)	0.08541
Calculation of ^{144}Nd corrected for Sm interference including a mass bias factor from Sm		
$R^{Sm}{}_M$	$^{147}Sm_M/^{149}Sm_M$	1.06040
Y_M	Y_T*([$R^{Sm}{}_M/R^{Sm}{}_T$]^a1)	5.05125
^{144}Sm	$^{147}Sm_M/(^{147}Sm/^{144}Sm)$	0.01793
^{144}Nd	$^{144}(Nd+Sm)_{M-}{}^{144}Sm$	1.901
Calculation of ^{143}Nd/^{144}Nd corrected for mass fractionation		
R_M	$^{146}Nd_M/^{144}Nd$	0.742499
X_T	$X_M/([R_M/R_T]$^a2)	0.511727

Table 2: Step-by-step calculation of the true ^{143}Nd/^{144}Nd ratio for method 2



Isotope Ratios

Ratio	Isotope1	Isotope2	IEC	Norm1	Norm2
1	1:143Nd	1:144Nd	x	x	
2	1:146Nd	1:144Nd	x		
3	1:147Sm	1:149Sm			

Interference Correction

Interf.	Ratio	Corr.Val.	Norm1	Norm2
Sm	147/144	4.87710		x

☑ Mass Bias Correction

Normalizing Ratio 1: 1:146Nd/1:144N
Normalizing Ratio 2: 1:147Sm/1:149S
Correction Law: Exponential Law
True Value 1: 0.7219
True Value 2: 1.08507

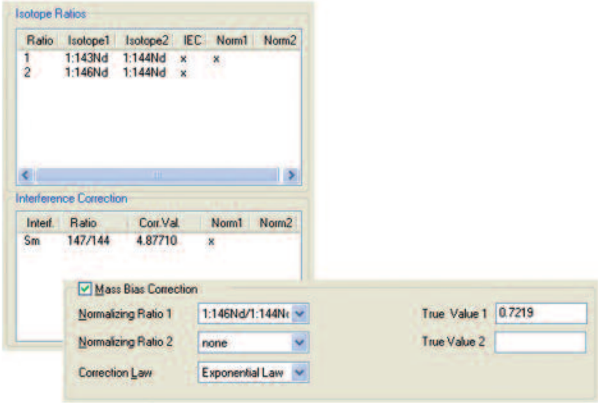
Figure 2: Screenshot of the Method Editor (evaluation pane) for method 2

^{143}Nd/^{144}Nd is interference corrected (IEC) using the ^{147}Sm/^{144}Sm ratio corrected for mass bias using Normalizing Ratio 2 (^{147}Sm/^{149}Sm = true ratio). The ^{143}Nd/^{144}Nd ratio is then corrected for mass fractionation using Normalizing Ratio 1 (^{146}Nd/^{144}Nd = 0.7219).

Method 3: Interference correction including a mass bias factor for Sm based on the measurement of ^{146}Nd/^{144}Nd

Variables	Description	Value
m1	mass ^{146}Nd	145.91311
m2	mass ^{144}Nd	143.91008
m3	mass ^{143}Nd	142.90981
m4	mass ^{144}Nd	143.91008
R_T	true ratio ^{146}Nd/^{144}Nd	0.7219
R_M	measured ratio ^{146}Nd/^{144}Nd	
X_T	true ratio ^{143}Nd/^{144}Nd	
X_M	measured ratio ^{143}Nd/^{144}Nd	
a2	ln[m3/m4]/ln[m1/m2]	-0.504603
m5	mass ^{147}Sm	146.91489
m6	mass ^{144}Sm	143.91199
Y_T	true ratio ^{147}Sm/^{144}Sm	4.87710
a1	ln(m5/m6)/ln(m1/m2)	1.49403
Measured Data		
$^{143}Nd_M$	measured intensity ^{143}Nd (V)	0.9592
$^{144}(Nd+Sm)_M$	measured intensity ^{144}(Nd+Sm) (V)	1.919
$^{146}Nd_M$	measured intensity ^{146}Nd (V)	1.412
$^{147}Sm_M$	measured intensity ^{147}Sm (V)	0.09056
Calculation of ^{144}Nd corrected for Sm interference including a mass bias factor from Nd		
^{144}Sm	$^{147}Sm_M/Y_T$	0.018569
^{144}Nd	$^{144}(Nd+Sm)_{M-}{}^{144}Sm$	1.90059
R_M	$^{146}Nd_M/^{144}Nd$	0.742749
STEP 1		
$^{147}Sm/^{144}Sm_{step1}$	Y_T*(R_M/R_T)^a1	5.089032
$^{144}Sm_1$	$^{147}Sm_M/(^{147}Sm/^{144}Sm_{step1})$	0.0177959
$^{144}Nd_1$	$^{144}(Nd+Sm)_{M-}{}^{144}Sm_1$	1.901358
$^{146}Nd/^{144}Nd_{step1}$	$^{146}Nd_M/^{144}Nd_1$	0.742447
STEP 2		
$^{147}Sm/^{144}Sm_{step2}$	Y_T*$(^{146}Nd/^{144}Nd_{step1}/R_T)$^a1	5.085940
$^{144}Sm_2$	$^{147}Sm_M/(^{147}Sm/^{144}Sm_{step2})$	0.0178068
$^{144}Nd_2$	$^{144}(Nd+Sm)_{M-}{}^{144}Sm_2$	1.901348
$^{146}Nd/^{144}Nd_{step2}$	$^{146}Nd_M/^{144}Nd_2$	0.742451
STEP 3		
$^{147}Sm/^{144}Sm_{step3}$	Y_T*$(^{146}Nd/^{144}Nd_{step2}/R_T)$^a1	5.085983
$^{144}Sm_3$	$^{147}Sm_M/(^{147}Sm/^{144}Sm_{step3})$	0.0178066
$^{144}Nd_3$	$^{144}(Nd+Sm)_{M-}{}^{144}Sm_3$	1.901348
$^{146}Nd/^{144}Nd_{step3}$	$^{146}Nd_M/^{144}Nd_3$	0.742451
STEP 4		
$^{147}Sm/^{144}Sm_{step4}$	Y_T*$(^{146}Nd/^{144}Nd_{step3}/R_T)$^a1	5.085982
$^{144}Sm_4$	$^{147}Sm_M/(^{147}Sm/^{144}Sm_{step4})$	0.0178066
$^{144}Nd_4$	$^{144}(Nd+Sm)_{M-}{}^{144}Sm_4$	1.901348
$^{146}Nd/^{144}Nd_{step4}$	$^{146}Nd_M/^{144}Nd_4$	0.742451
STEP 5		
$^{147}Sm/^{144}Sm_{step5}$	Y_T*$(^{146}Nd/^{144}Nd_{step4}/R_T)$^a1	5.085982
$^{144}Sm_5$	$^{147}Sm_M/(^{147}Sm/^{144}Sm_{step5})$	0.0178066
$^{144}Nd_5$	$^{144}(Nd+Sm)_{M-}{}^{144}Sm_5$	1.901348
$^{146}Nd/^{144}Nd_{step5}$	$^{146}Nd_M/^{144}Nd_5$	0.742451
X_M	$^{143}Nd_M/^{144}Nd_5$	
Calculation of ^{143}Nd/^{144}Nd corrected for mass fractionation		
X_T	X_M*$([^{146}Nd/^{144}Nd_{step5}/R_T]$^a2)	0.511677

Table 3: Step-by-step calculation of the true ^{143}Nd/^{144}Nd ratio for method 3



Isotope Ratios

Ratio	Isotope1	Isotope2	IEC	Norm1	Norm2
1	1:143Nd	1:144Nd	x	x	
2	1:146Nd	1:144Nd	x		

Interference Correction

Interf.	Ratio	Corr.Val.	Norm1	Norm2
Sm	147/144	4.87710	x	

☑ Mass Bias Correction

Normalizing Ratio 1 1:146Nd/1:144N

True Value 1 0.7219

Normalizing Ratio 2 none

True Value 2

Correction Law Exponential Law

Figure 3: Screenshot of the Method Editor (evaluation pane) for method 3

^{143}Nd/^{144}Nd is interference corrected (IEC) using the ^{147}Sm/^{144}Sm ratio corrected for mass bias using Normalizing Ratio 1 (^{146}Nd/^{144}Nd). The ^{143}Nd/^{144}Nd ratio is then corrected for mass fractionation using Normalizing Ratio 1 (^{146}Nd/^{144}Nd = 0.7219).

Results

The ^{143}Nd/^{144}Nd ratio of Merck is 0.511728 ± 20 ppm (1RSD), based on measurements made on more than 50 NEPTUNEs in the Bremen factory. Of the three methods discussed here, the most accurate ^{143}Nd/^{144}Nd ratio is obtained by method 2 (^{143}Nd/^{144}Nd = 0.511727 ± 11 ppm), where the mass bias of Sm was determined during the measurement and taken into account for the interference correction. The ^{143}Nd/^{144}Nd ratio obtained by method 1 is off by more than 600 ppm. The ratio is too high due to an overcorrection of the ^{144}Sm on the measured 144 intensity. The ^{143}Nd/^{144}Nd ratio obtained by method 3 is too low by 100 ppm, which results from the fact that the mass bias from Nd is not exactly the same as that of Sm.

	^{143}Nd/^{144}Nd	1sigma (ppm)
Accepted	0.511728	20
Method 1	0.512046	11
Method 2	0.511727	11
Method 3	0.511677	10

Table 4: The accepted ^{143}Nd/^{144}Nd compared with the ^{143}Nd/^{144}Nd ratios obtained by the three different methods (Merck solution)

Summary

Three methods for performing interference corrections using the multicollector software of the Thermo Scientific NEPTUNE MC-ICP-MS have been illustrated. The examples show the importance of performing accurate interference corrections in case where there is a significant amount of the interfering element. These corrections are best done by taking into account a mass bias factor, ideally from the interfering element itself.

Acknowledgements

We thank Dr. Geoff Nowell from the University of Durham for sharing his strategy on performing off-line interference corrections.

References

G.M. Nowell, D.G. Pearson, C.J. Ottey, J. Schwieters & D. Dowall (2003) Long-term performance characteristics of a plasma ionization Multi-Collector Mass Spectrometer (PIMSS): the Thermo Scientific Neptune. In: Plasma Source Mass Spectrometry, Applications and Emerging Technologies, eds. J.G. Holland & S.D. Tanner. Royal Society of Chemistry Special Publication, 307-320.

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