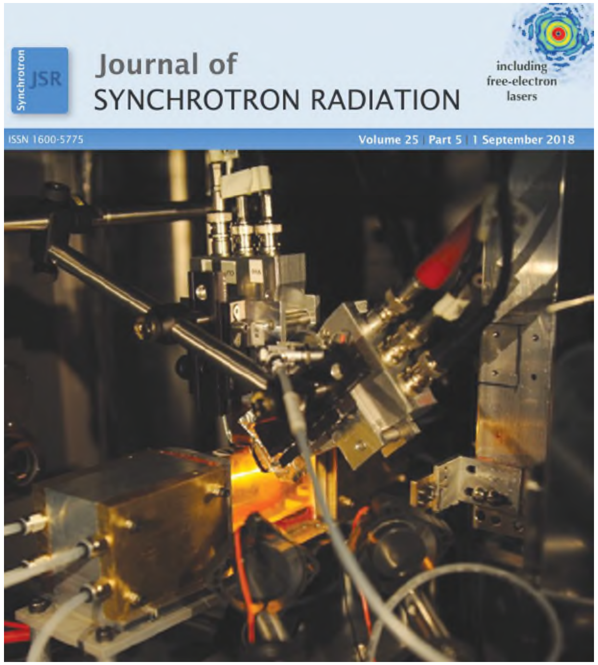
Introduction to isotope fractionation and SciPhon

Justin Hu



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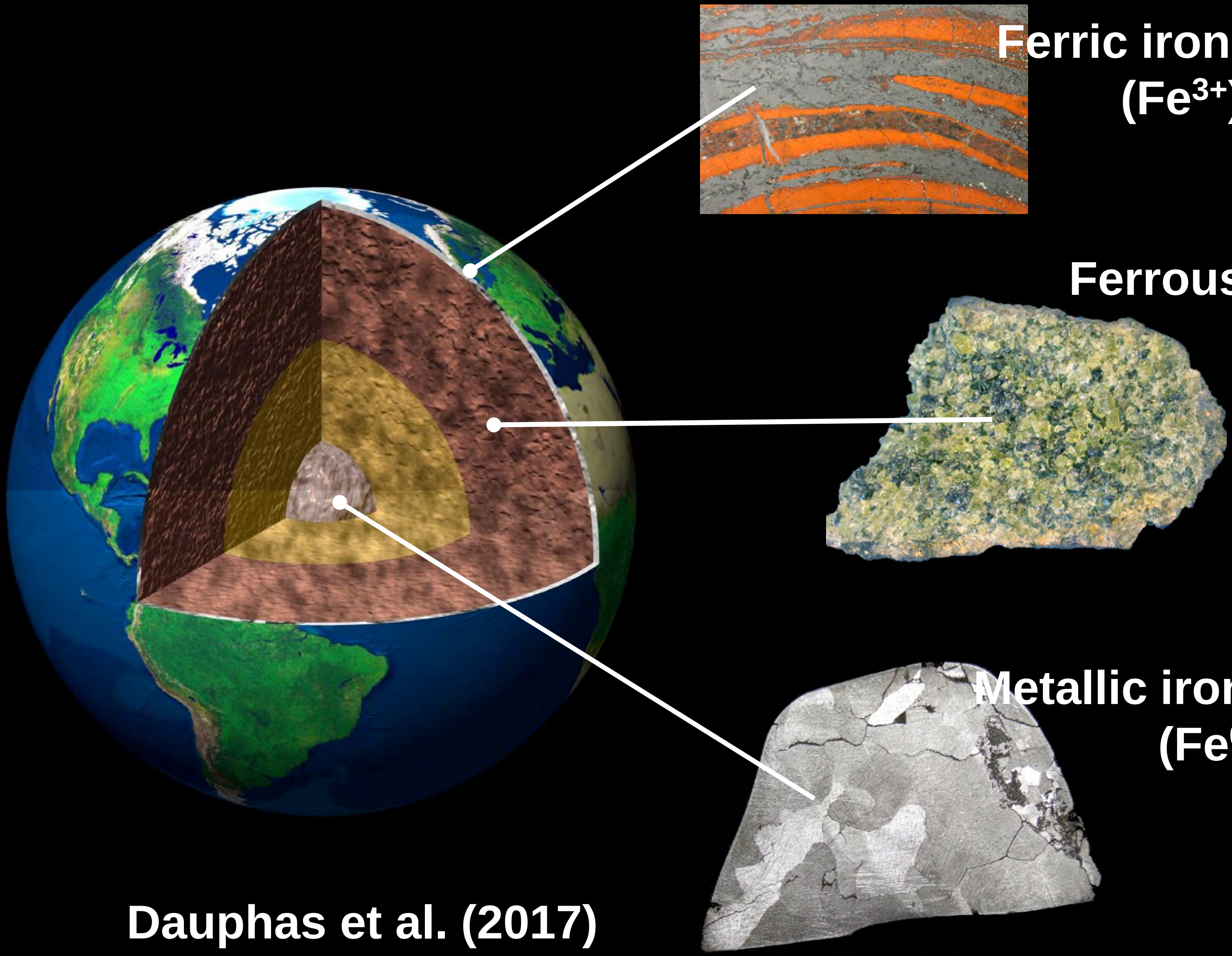
The University of Chicago



Ferric iron
(Fe^{3+})

Ferrous iron
(Fe^{2+})

Metallic iron
(Fe^{0})

Dauphas et al. (2017)

Primer on isotopic fractionation

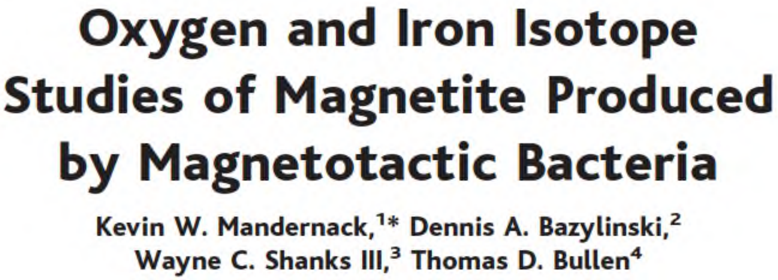
$$\delta^{56}\mathrm{Fe}=\left[\frac{\left({}^{56}\mathrm{Fe}/{}^{54}\mathrm{Fe}\right)_{\mathrm{sample}}}{\left({}^{56}\mathrm{Fe}/{}^{54}\mathrm{Fe}\right)_{\mathrm{standard}}}-1\right]\times 1000$$

δ^{56}Fe is the deviation in part permil of the ^{56}Fe/^{54}Fe ratio of a sample relative to that of some reference material

Example:
15.6994 *vs*. 15.6979
=0.1‰ fractionation

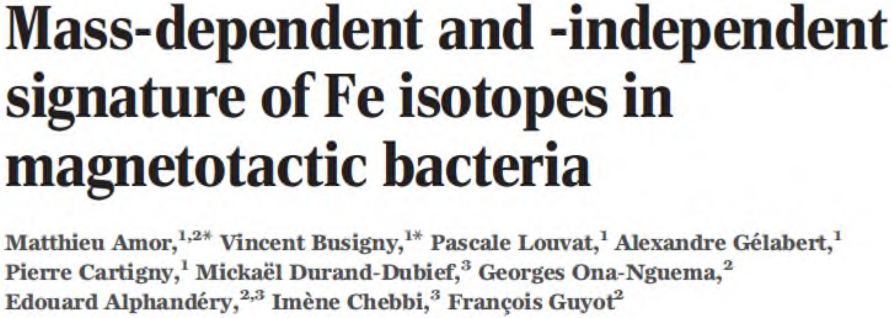
Dauphas & Rouxel (2006) Mass spectrometry and natural variations of iron isotopes. Mass Spectrom. Rev. 25, 515-550.

Uses of iron isotopes



Oxygen and Iron Isotope Studies of Magnetite Produced by Magnetotactic Bacteria

Kevin W. Mandernack,[1]* Dennis A. Bazylinski,[2]
Wayne C. Shanks III,[3] Thomas D. Bullen[4]

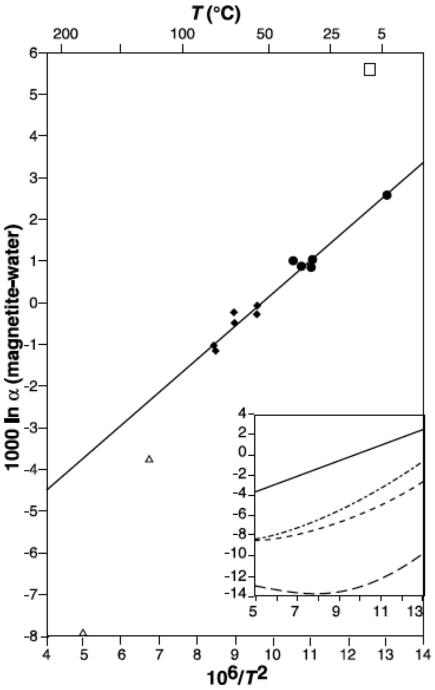


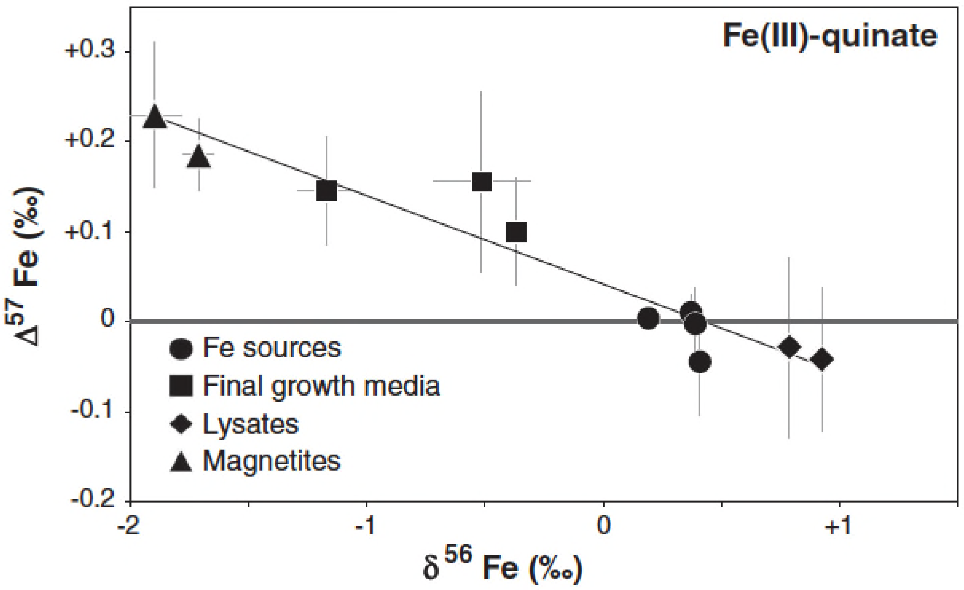
Mass-dependent and -independent signature of Fe isotopes in magnetotactic bacteria

Matthieu Amor,[1,2]* Vincent Busigny,[1]* Pascale Louvat,[1] Alexandre Gélabert,[1]
Pierre Cartigny,[1] Mickaël Durand-Dubief,[3] Georges Ona-Nguema,[2]
Edouard Alphandéry,[2,3] Imène Chebbi,[3] François Guyot[2]

Science 1999

Science 2016



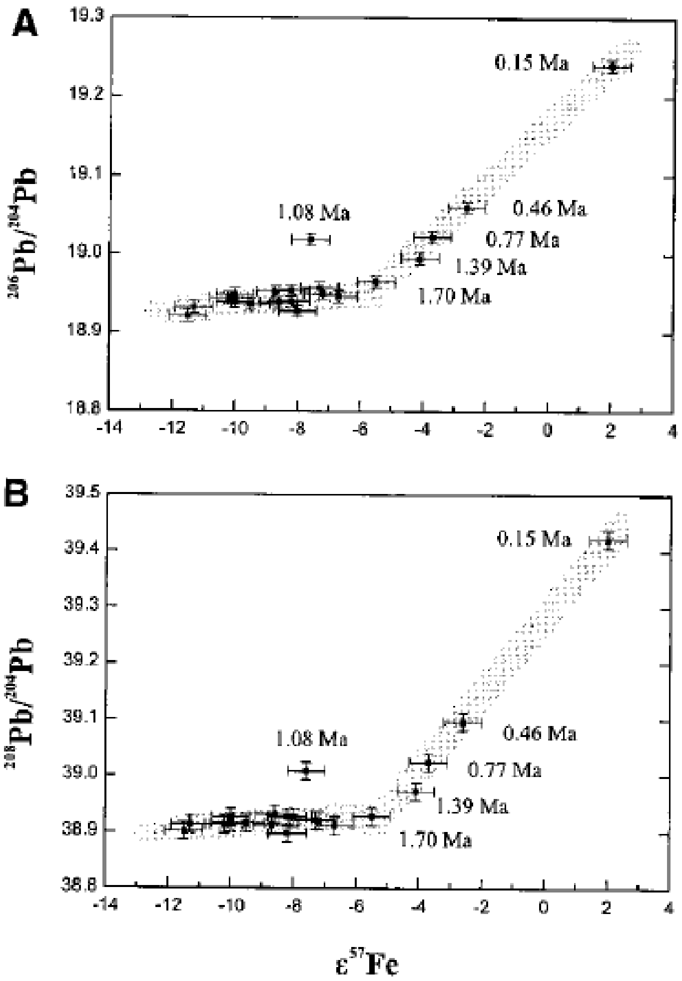


Uses of iron isotopes

Secular Variation of Iron Isotopes in North Atlantic Deep Water

Xiang-Kun Zhu,* R. Keith O'Nions, Yueling Guo, Ben C. Reynolds

Science 2000

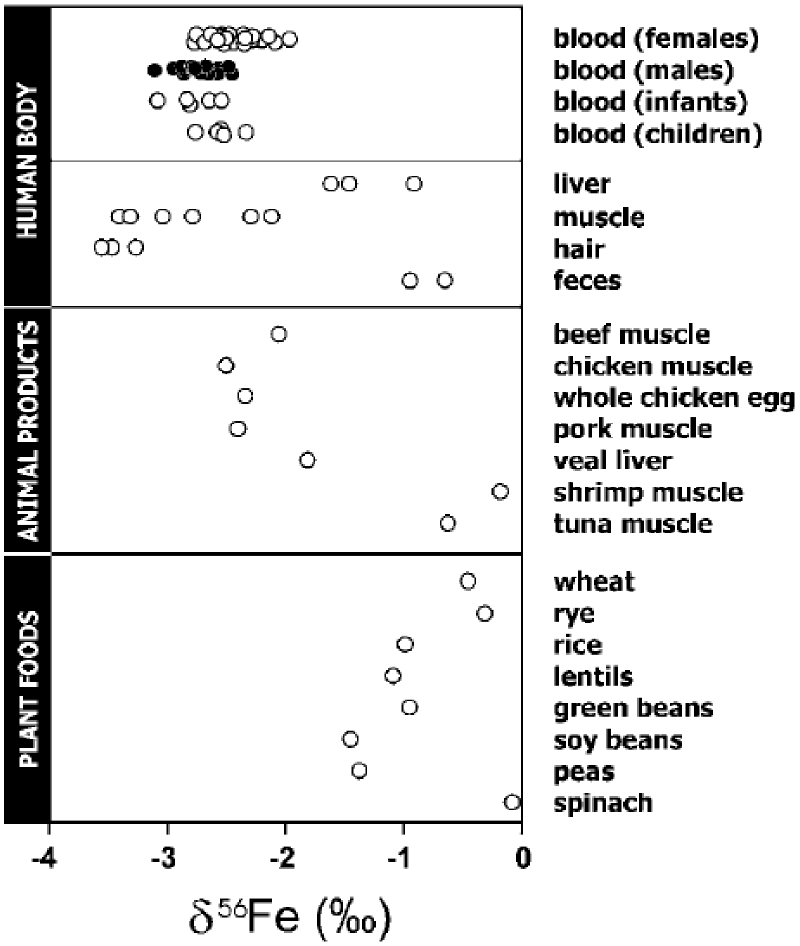


Uses of iron isotopes

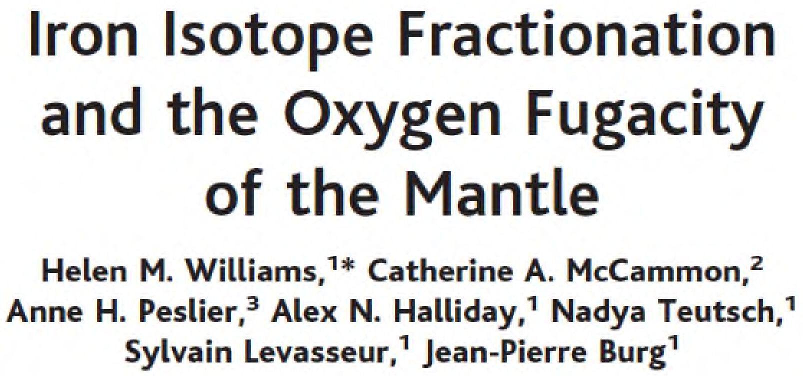
Natural Iron Isotope Variations in Human Blood

Thomas Walczyk[1]* and Friedhelm von Blanckenburg[2]†

Science 2002



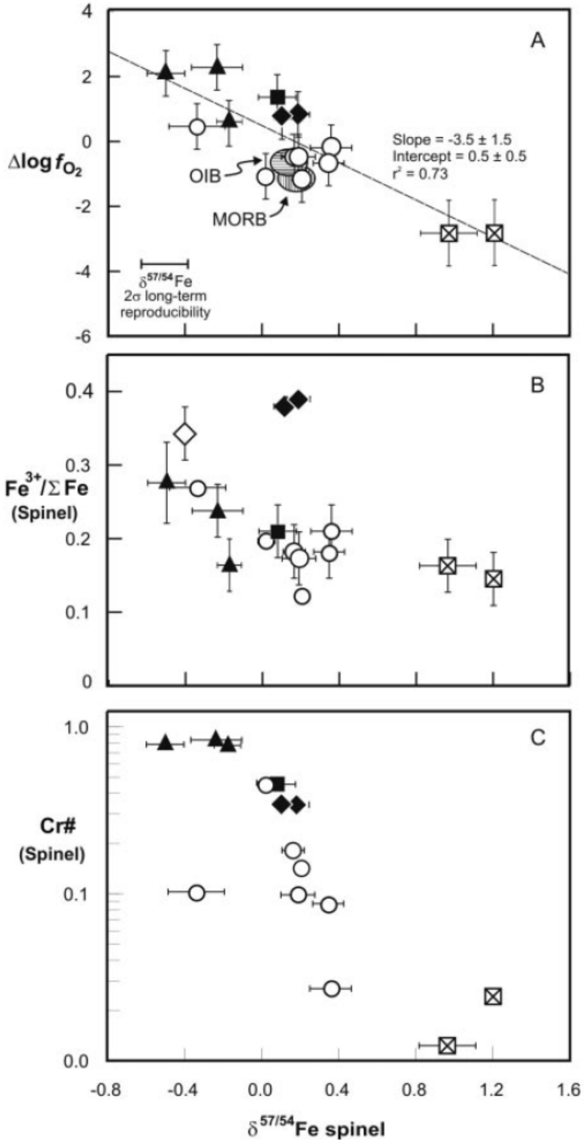
Uses of iron isotopes



Iron Isotope Fractionation and the Oxygen Fugacity of the Mantle

Helen M. Williams,[1]* Catherine A. McCammon,[2]
Anne H. Peslier,[3] Alex N. Halliday,[1] Nadya Teutsch,[1]
Sylvain Levasseur,[1] Jean-Pierre Burg[1]

Science 2004

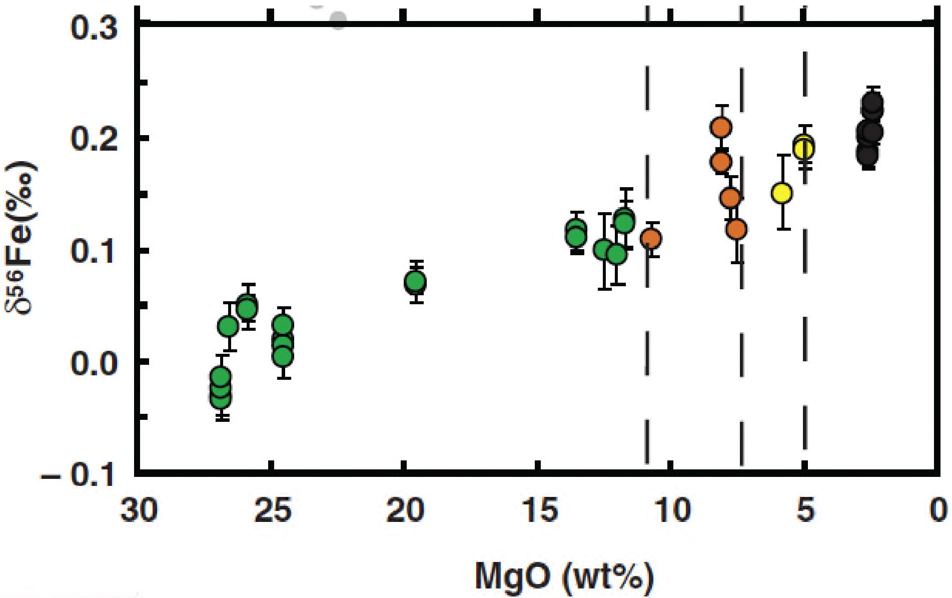


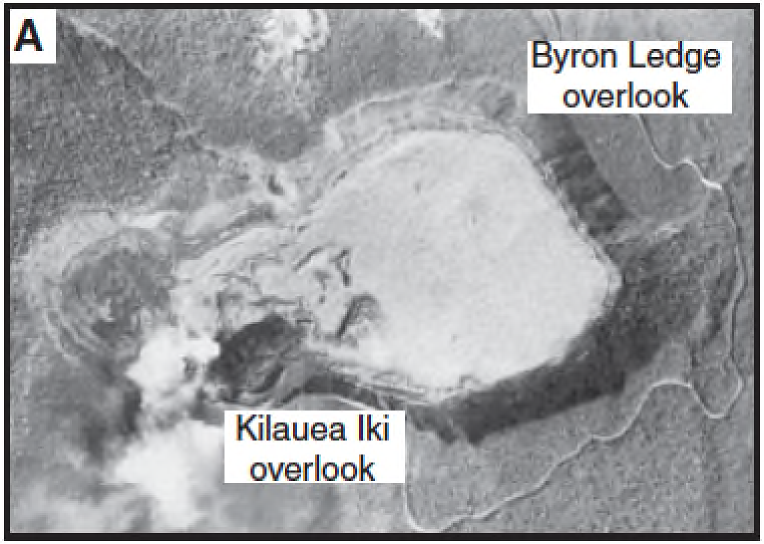
Uses of iron isotopes

Iron Isotope Fractionation During Magmatic Differentiation in Kilauea Iki Lava Lake

Fang-Zhen Teng,[1]*† Nicolas Dauphas,[1] Rosalind T. Helz[2]

Science 2008



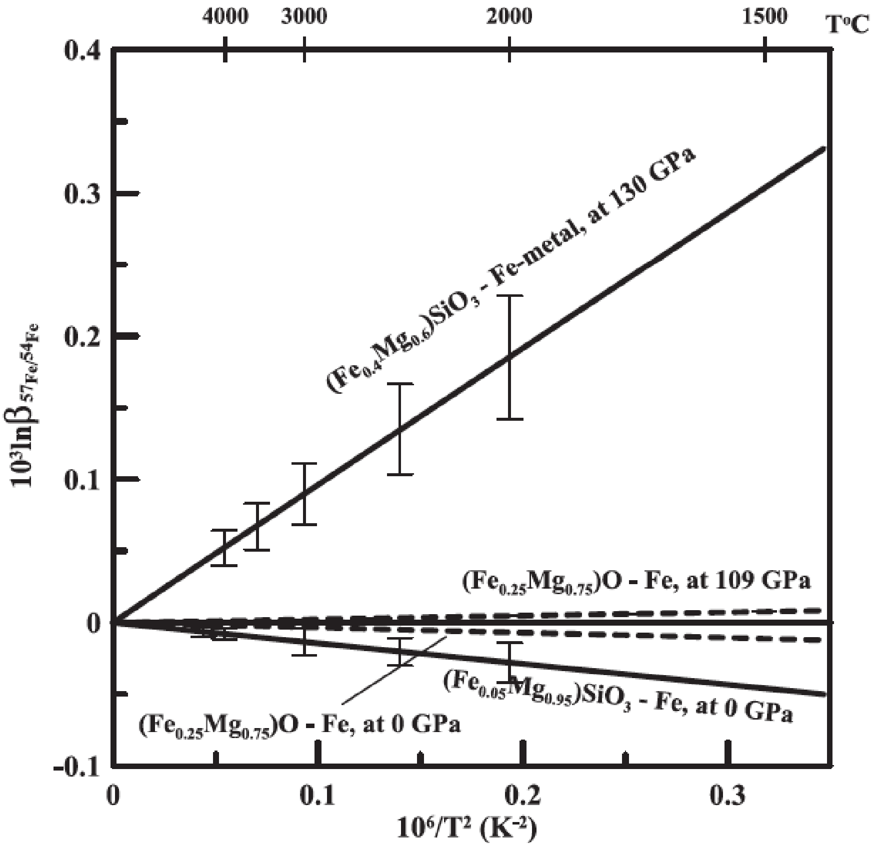


Uses of iron isotopes

Equilibrium Iron Isotope Fractionation at Core-Mantle Boundary Conditions

Veniamin B. Polyakov

Science 2009

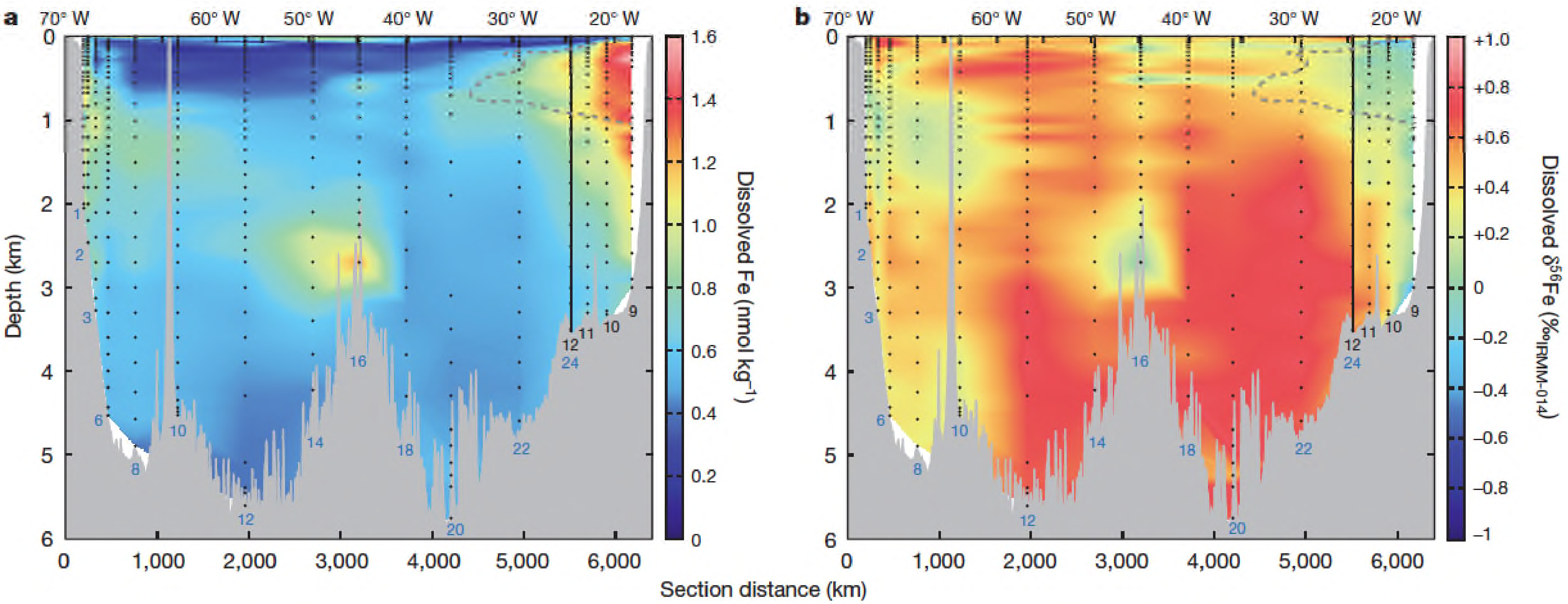


Uses of iron isotopes

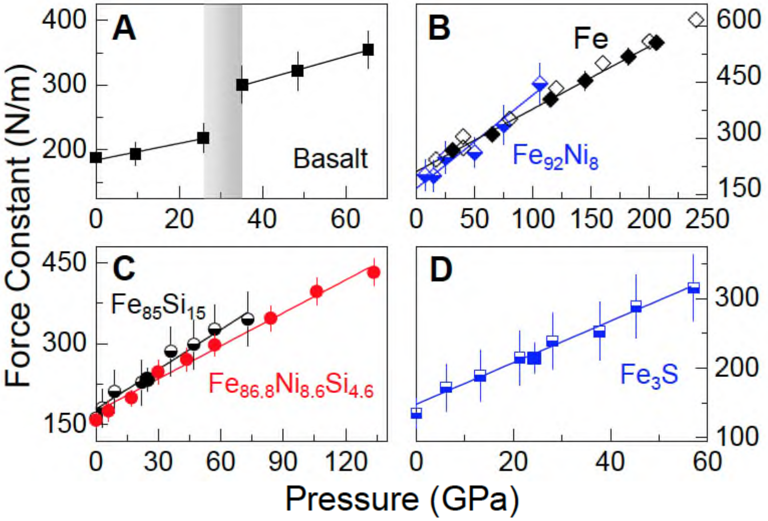
Quantification of dissolved iron sources to the North Atlantic Ocean

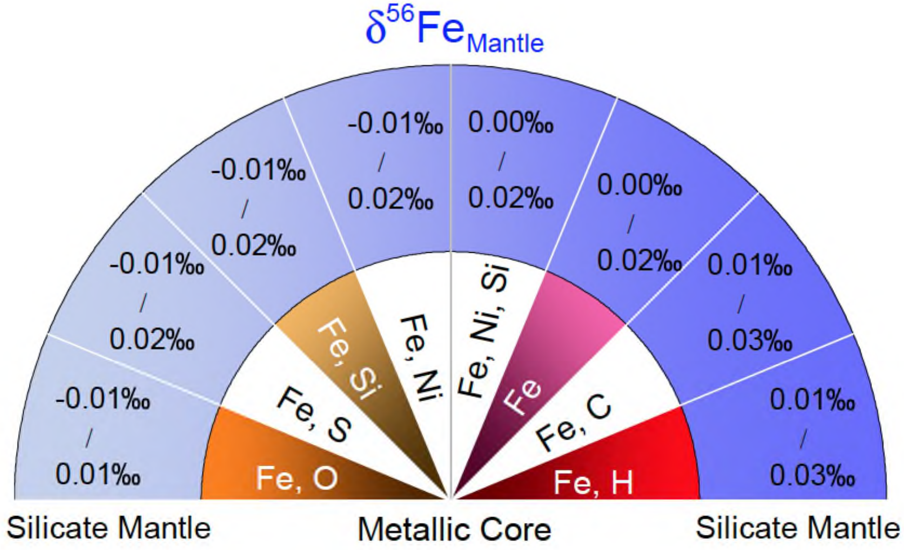
Tim M. Conway[1]† & Seth G. John[1]

Nature 2014



Uses of iron isotopes





Nature Communications 2016

Iron isotopic fractionation between silicate mantle and metallic core at high pressure

Jin Liu[1,w], Nicolas Dauphas[2], Mathieu Roskosz[3], Michael Y. Hu[4], Hong Yang[5], Wenli Bi[4,6], Jiyong Zhao[4], Esen E. Alp[4], Justin Y. Hu[2] & Jung-Fu Lin[1,5]

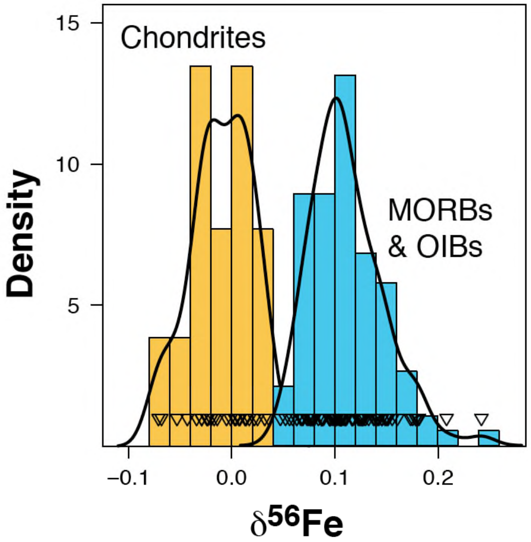
Science 2016

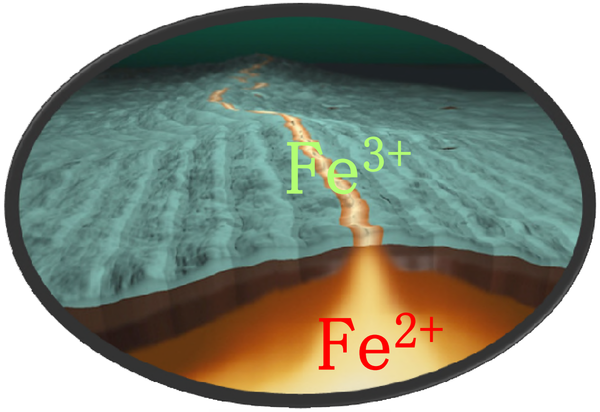
Pressure-dependent isotopic composition of iron alloys

A. Shahar,[1]* E. A. Schauble,[2] R. Caracas,[3] A. E. Gleason,[4] M. M. Reagan,[5] Y. Xiao,[6] J. Shu,[1] W. Mao[5]

Motivation

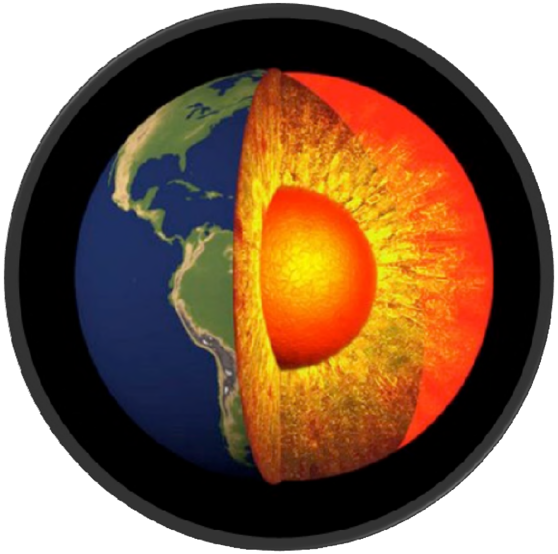
Teng *et al.* 13





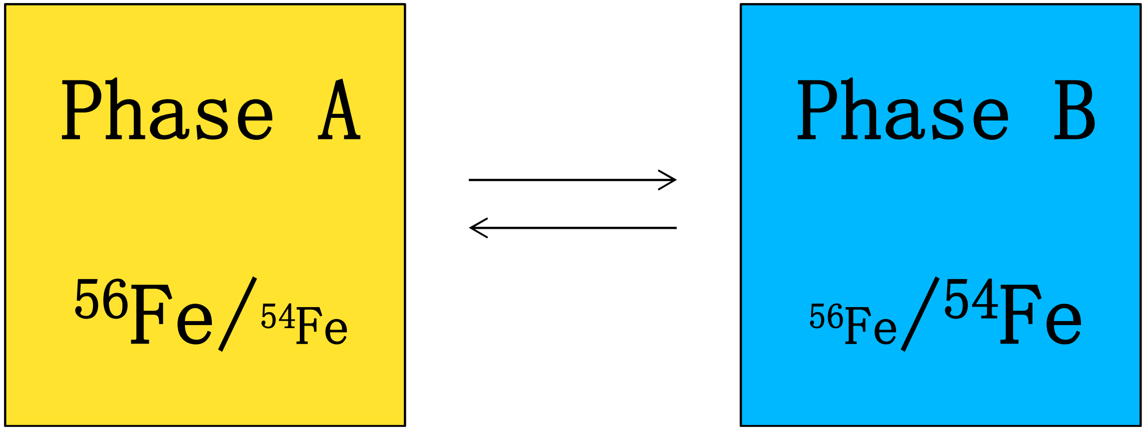
Mantle melting
(Williams *et al.* 05, Weyer & Ionov 07,
Dauphas *et al.* 09)

Evaporation
(Poitrasson *et al.* 04)



Metal-silicate partitioning
(Polyakov 09)

Equilibrium isotopic fractionation



Phase A

$^{56}Fe/^{54}Fe$

Phase B

$^{56}Fe/^{54}Fe$

How do iron isotopes partition between coexisting phases at equilibrium?

Equilibrium isotopic fractionation

FeX *vs.* $\mathrm{Fe_g}$

$$^{56}\mathrm{Fe_g} + {}^{54}\mathrm{FeX} \rightleftharpoons {}^{54}\mathrm{Fe_g} + {}^{56}\mathrm{FeX}$$

$$\mathrm{K_{eq}} = \frac{\left[{}^{54}\mathrm{Fe_g}\right]\left[{}^{56}\mathrm{FeX}\right]}{\left[{}^{56}\mathrm{Fe_g}\right]\left[{}^{54}\mathrm{FeX}\right]} = \frac{\left[{}^{56}\mathrm{FeX}\right]/\left[{}^{54}\mathrm{FeX}\right]}{\left[{}^{56}\mathrm{Fe_g}\right]/\left[{}^{54}\mathrm{Fe_g}\right]} = \frac{\left({}^{56}\mathrm{Fe}/{}^{54}\mathrm{Fe}\right)_{\mathrm{FeX}}}{\left({}^{56}\mathrm{Fe}/{}^{54}\mathrm{Fe}\right)_{\mathrm{Fe_g}}}$$

$$\mathrm{K_{eq}} = e^{\frac{-\Delta_R G}{RT}}$$

$$\mathrm{K_{eq}} = e^{\frac{-\Delta \mathrm{F}}{RT}}$$

$$F = -RT \ln(Q_{\mathrm{trans}} \times Q_{\mathrm{rot}} \times Q_{\mathrm{vib}})$$

$$\mathrm{K_{eq}} = e^{\sum_{\mathrm{products}}(Q_{\mathrm{trans}} \times Q_{\mathrm{rot}} \times Q_{\mathrm{vib}}) - \sum_{\mathrm{reactants}}(Q_{\mathrm{trans}} \times Q_{\mathrm{rot}} \times Q_{\mathrm{vib}})}$$

$$\mathrm{K_{eq}} = \frac{\prod_{\mathrm{products}} Q_{\mathrm{trans}} \times Q_{\mathrm{rot}} \times Q_{\mathrm{vib}}}{\prod_{\mathrm{reactants}} Q_{\mathrm{trans}} \times Q_{\mathrm{rot}} \times Q_{\mathrm{vib}}}$$

Urey (1947); Bigeleisen and Mayer (1947)

Equilibrium isotopic fractionation

$$Q_{\mathrm{vib},i} = \frac{e^{-\frac{h\upsilon_i}{2kT}}}{1 - e^{-\frac{h\upsilon_i}{kT}}}$$

$$\mathrm{K_{eq}} = \prod_i \frac{u_i'}{u_i} \frac{e^{-u_i'/2}}{1 - e^{-u_i'}} \frac{1 - e^{-u_i}}{e^{-u_i/2}}$$

$$u_i = \frac{h\upsilon_i}{kT}$$

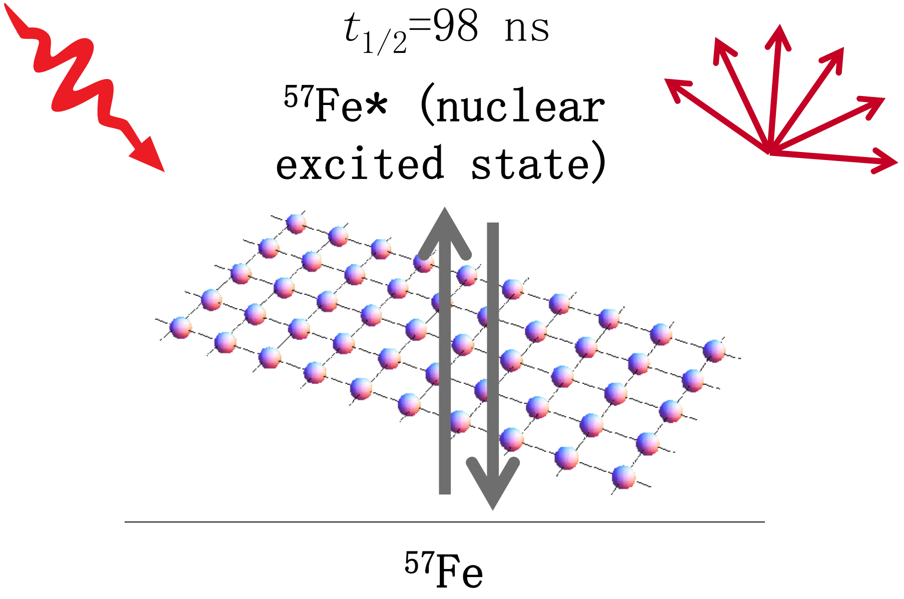
Equilibrium isotopic fractionation between a chemical compound and monoatomic gas is called the reduced partition function ratio and can be calculated from the vibration energies of the isotopic species

Reduced partition function ratio = β

Urey (1947); Bigeleisen and Mayer (1947)

NRIXS=Nuclear Resonant Inelastic X-ray Scattering

Sturhahn *et al.* 95
Seto *et al.* 95



Synchrotron pulsed
X-ray source
14.4 keV

Scattered X-rays
detector

$t_{1/2}$=98 ns

^{57}Fe* (nuclear
excited state)

^{57}Fe

β-factors in solids
(for harmonic potential)

Ratio of the masses of the
isotopes involved (e.g., 56/54)

Iron partial phonon density
of states (PDOS)

$$\ln \beta_{I/I^*} = \frac{3}{2}\left(\frac{M}{M^*} - 1\right)\int_0^{E_{\max}}\left(\frac{E}{2kT} + \frac{E/kT}{e^{E/kT} - 1} - 1\right) g(E)\, dE$$

Temperature at which
one wants to calculate β

Polyakov et al. (2005)
Dauphas et al. (2012)

β-factors in solids

$$\ln \beta_{I/I^*} = \frac{3}{2}\left(\frac{M}{M^*} - 1\right)\int_0^{E_{\max}} \left(\frac{E}{2kT} + \frac{E/kT}{e^{E/kT} - 1} - 1\right) g(E)\, dE$$

To a very good approximation:

$$1000 \ln \beta_{I/I^*} \simeq 1000\left(\frac{M}{M^*} - 1\right)\left(\frac{m_2^g}{8k^2T^2} - \frac{m_4^g}{480k^4T^4} + \frac{m_6^g}{20{,}160k^6T^6}\right)$$

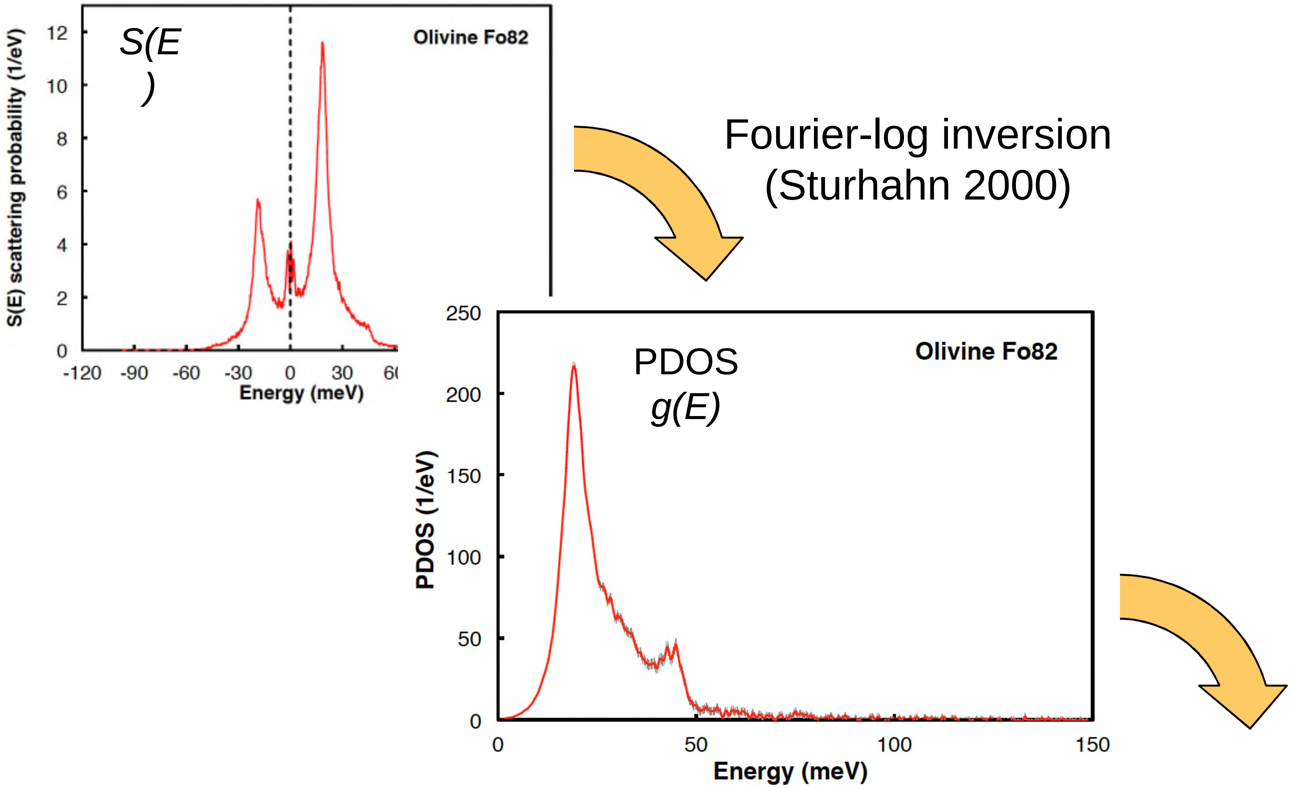
with

$$\boxed{m_j^g} = \int_0^{E_{\max}} E^j g(E)\, dE$$

j^th moment of g

Polyakov (2009)
Dauphas et al. (2012)

β−factors in solids

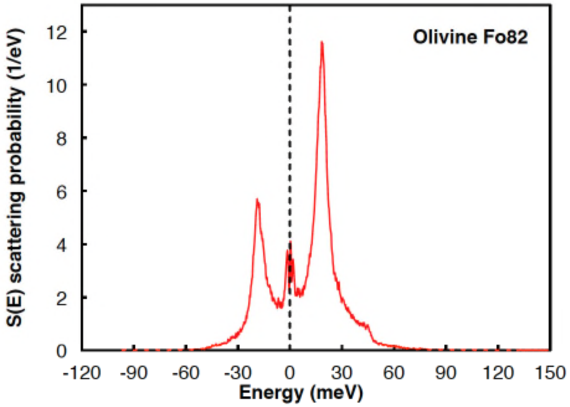


Fourier-log inversion
(Sturhahn 2000)

$$1000 \times \ln \beta_{I/I^*} \simeq 1000\left(\frac{M}{M^*}-1\right)\left(\frac{m_2^g}{8k^2T^2}-\frac{m_4^g}{480k^4T^4}+\frac{m_6^g}{20,160k^6T^6}\right)$$

β−factors in solids

Dauphas et al. (2012) and Hu et al. (2013) established relationships between the moments of S and g



$$1000\times\ln\beta_{I/I^*}=1000\left(\frac{M}{M^*}-1\right)$$

$$\times\frac{1}{E_r}\left[\frac{R_3^S}{8k^2T^2}-\frac{R_5^S-10R_2^SR_3^S}{480k^4T^4}+\frac{R_7^S+210(R_2^S)^2R_3^S-35R_3^SR_4^S-21R_2^SR_5^S}{20,160k^6T^6}\right]$$

$$R_j^S=\int_{-\infty}^{+\infty}S(E)(E-E_R)^j\mathrm{d}E$$

High temperature approximation

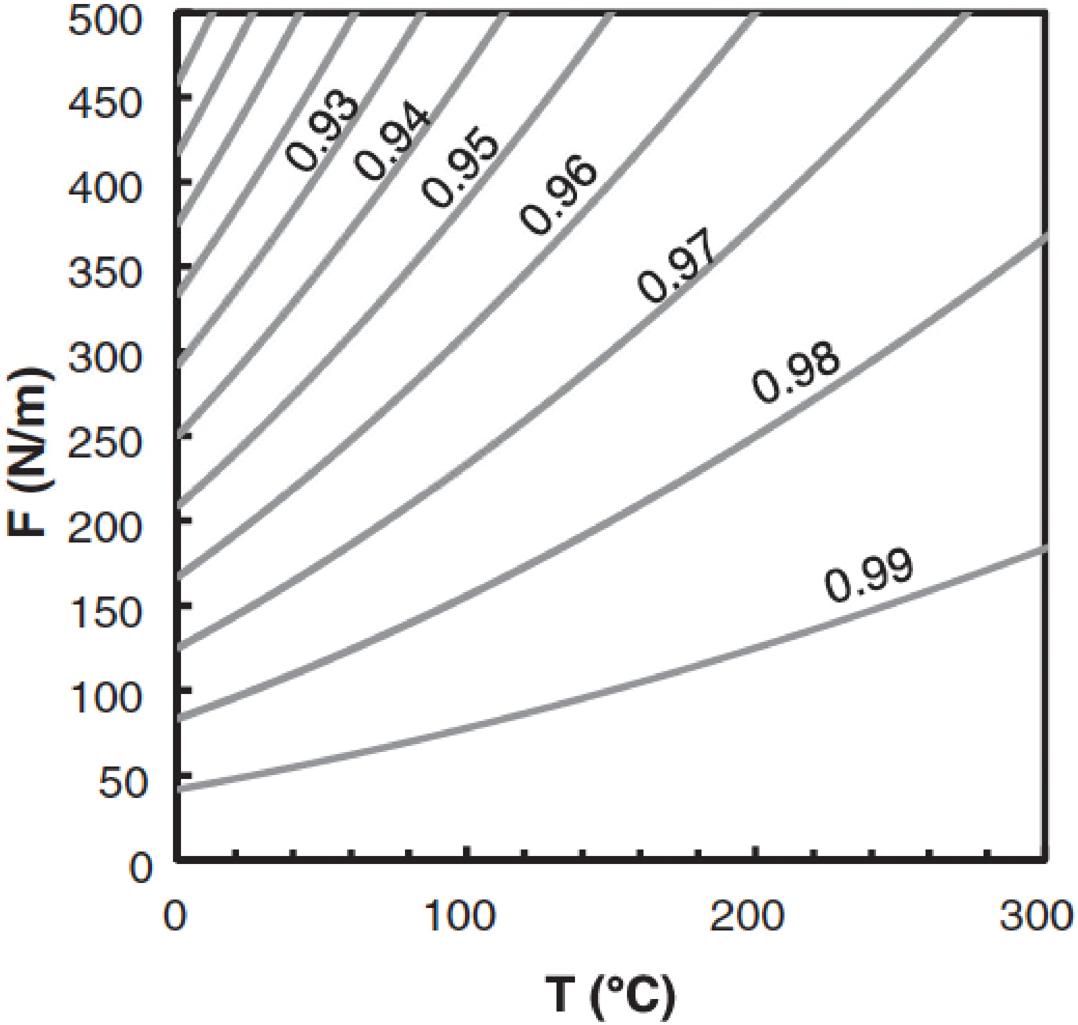
The sum rules of Lipkin (1995, 1999) identify the first terms with the mean force constant of iron bonds

$$1000 \times \ln\ \beta_{I/I^*} = 1000\left(\frac{1}{M^*} - \frac{1}{M}\right)\frac{\hbar^2}{8k^2T^2}\langle F\rangle$$

$$\langle F\rangle = \frac{M}{\hbar^2}\int_0^{+\infty} E^2 g(E)\mathrm{d}E = \frac{M}{E_R\hbar^2}\int_{-\infty}^{+\infty}(E - E_R)^3 S(E)\mathrm{d}E$$

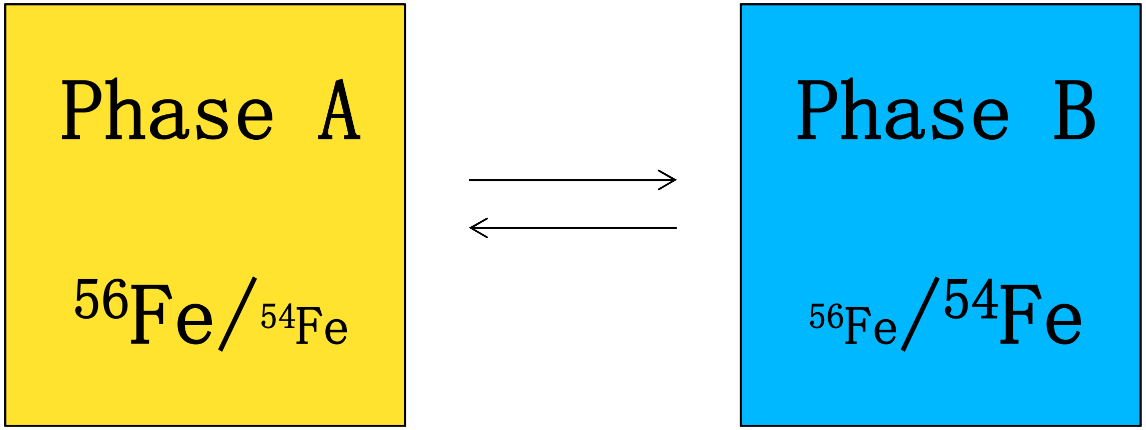
… a familiar formula in isotope geochemistry (Herzfeld and Teller, 1938; Bigeleisen and Mayer, 1947)

High temperature approximation



A good approximation for iron

Equilibration experiments



Phase A

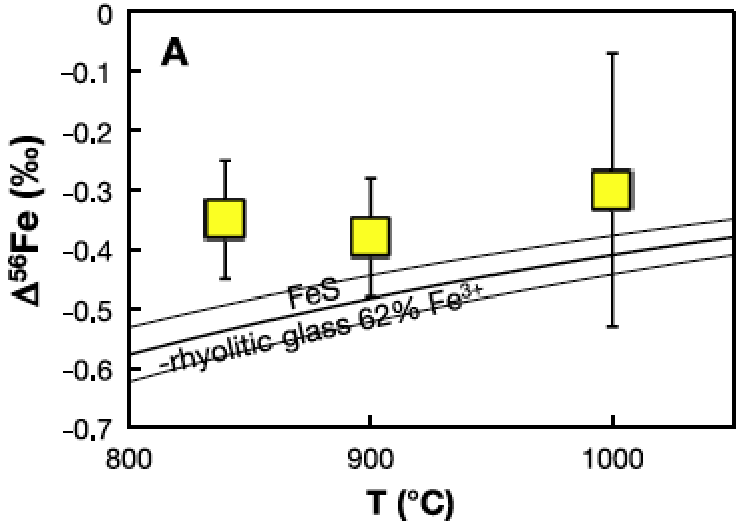
$^{56}Fe/^{54}Fe$

Phase B

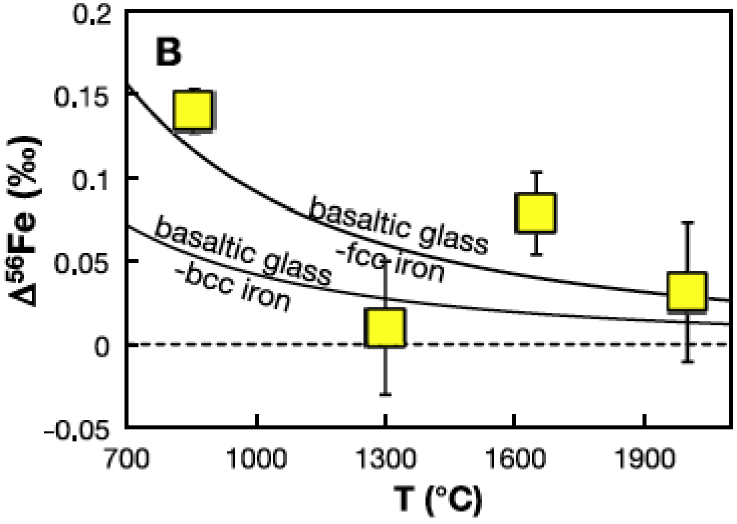
$^{56}Fe/^{54}Fe$

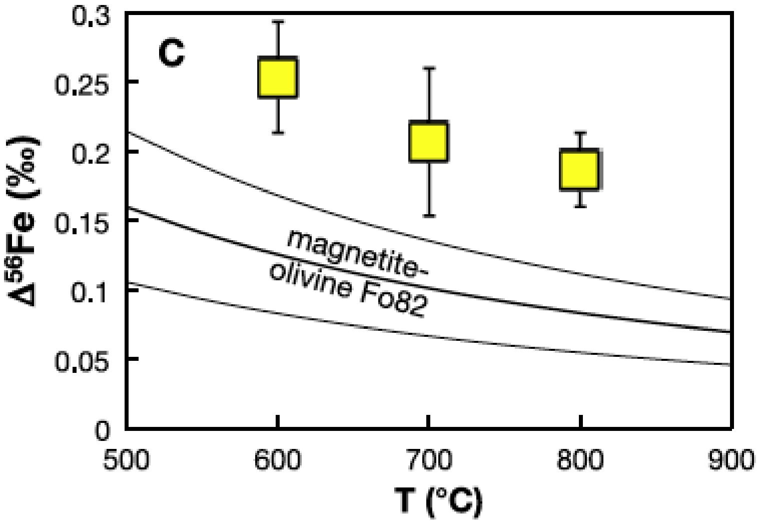
Method comparison

Data: Schuessler et al. (2007)
FC: Krawczynski et al. (2014), Dauphas et al. (2014)

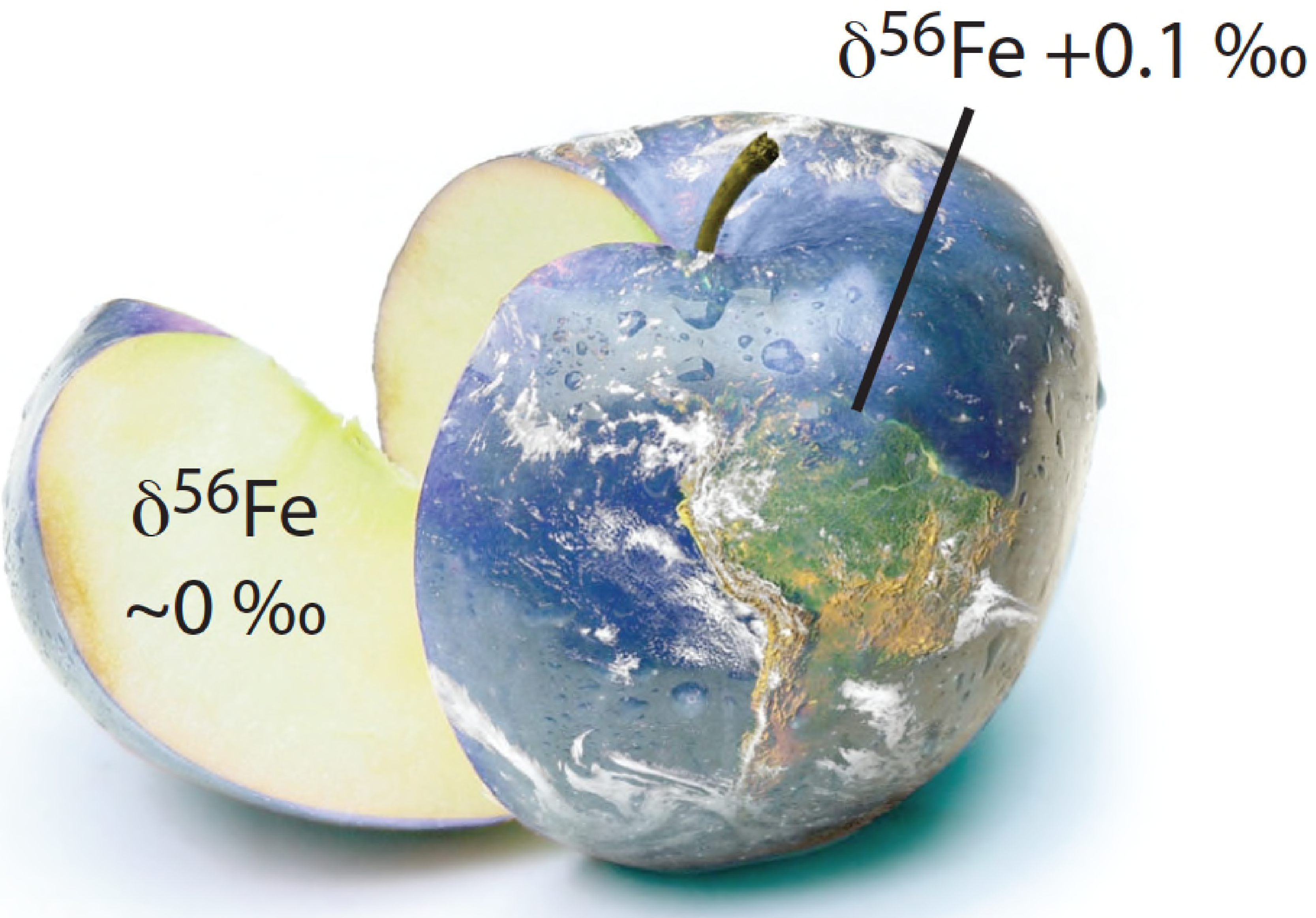


Data: Poitrasson et al. (2009), Hin et al. (2012),
Jordan and Young (2014), Shahar et al. (2013)
FC: Krawczynski et al. (2014), Dauphas et al. (2012)



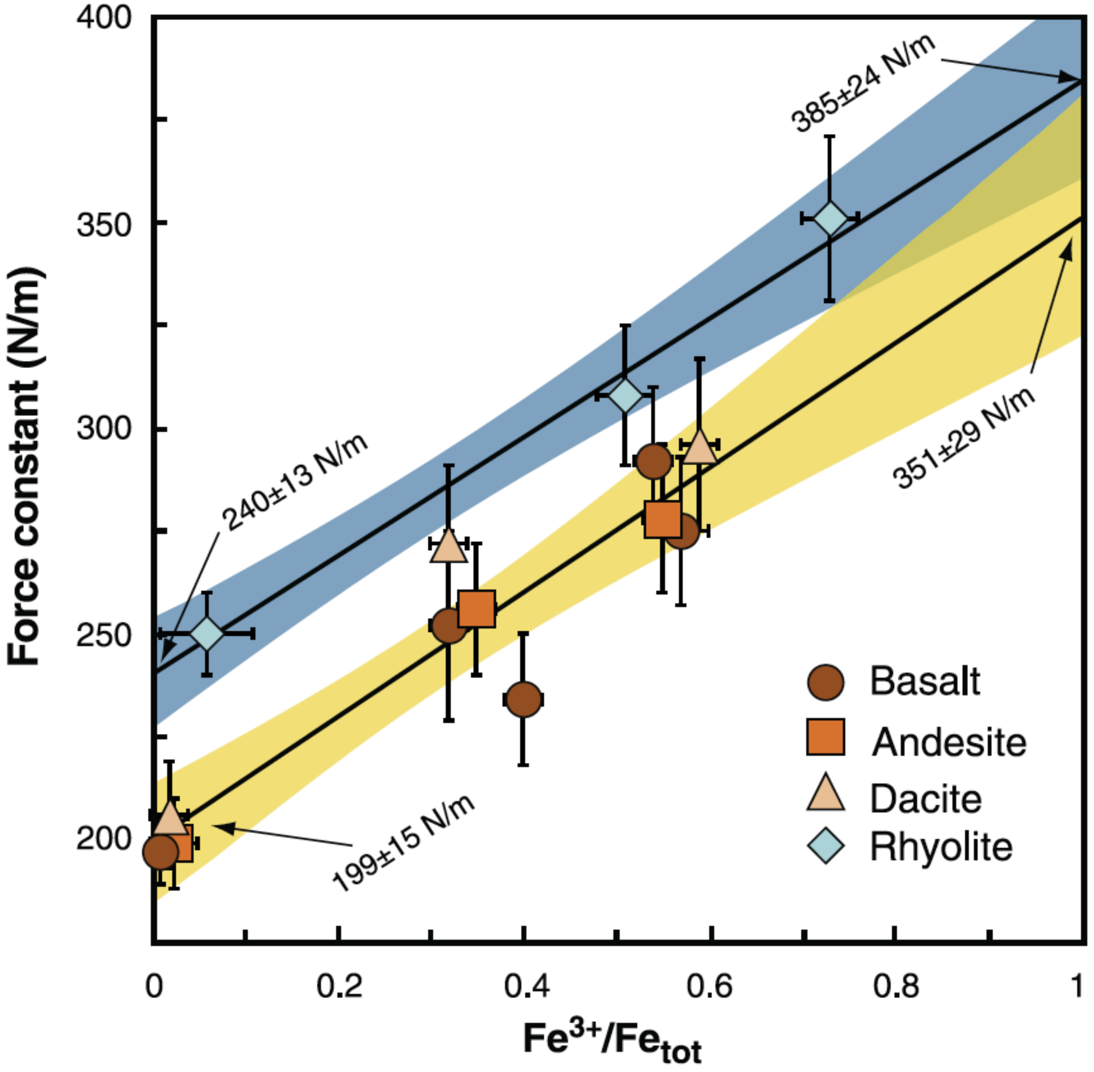


Data: Shahar et al. (2008)
FC: Polyakov et al. (2007), Dauphas et al. (2012, 2014)



Why does Earth's crust have different iron isotopic composition than the mantle, other planetary crusts, and chondrites?

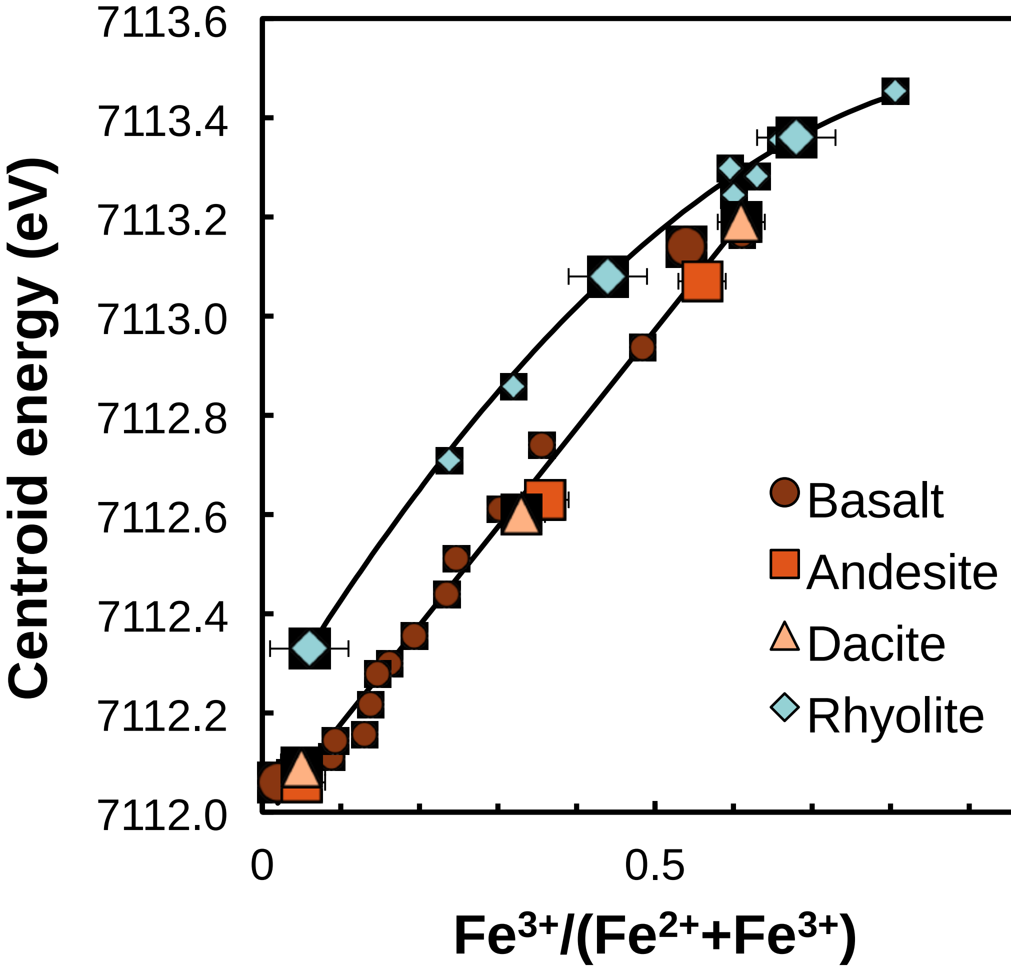
Force constant results



Dauphas et al. (2014)

Redox and structural controls in glasses

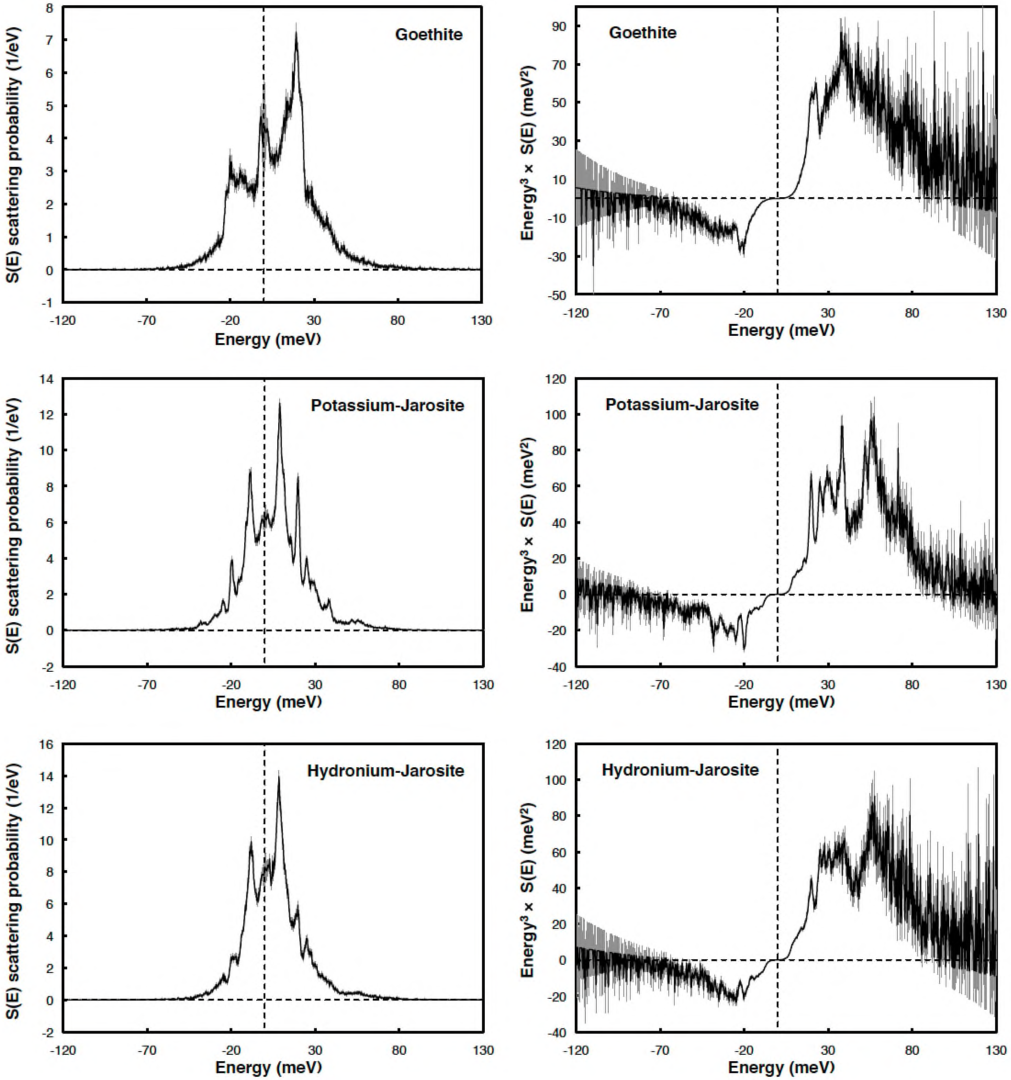
XANES



Cottrell *et al.* 09, Dauphas *et al.* (2014)

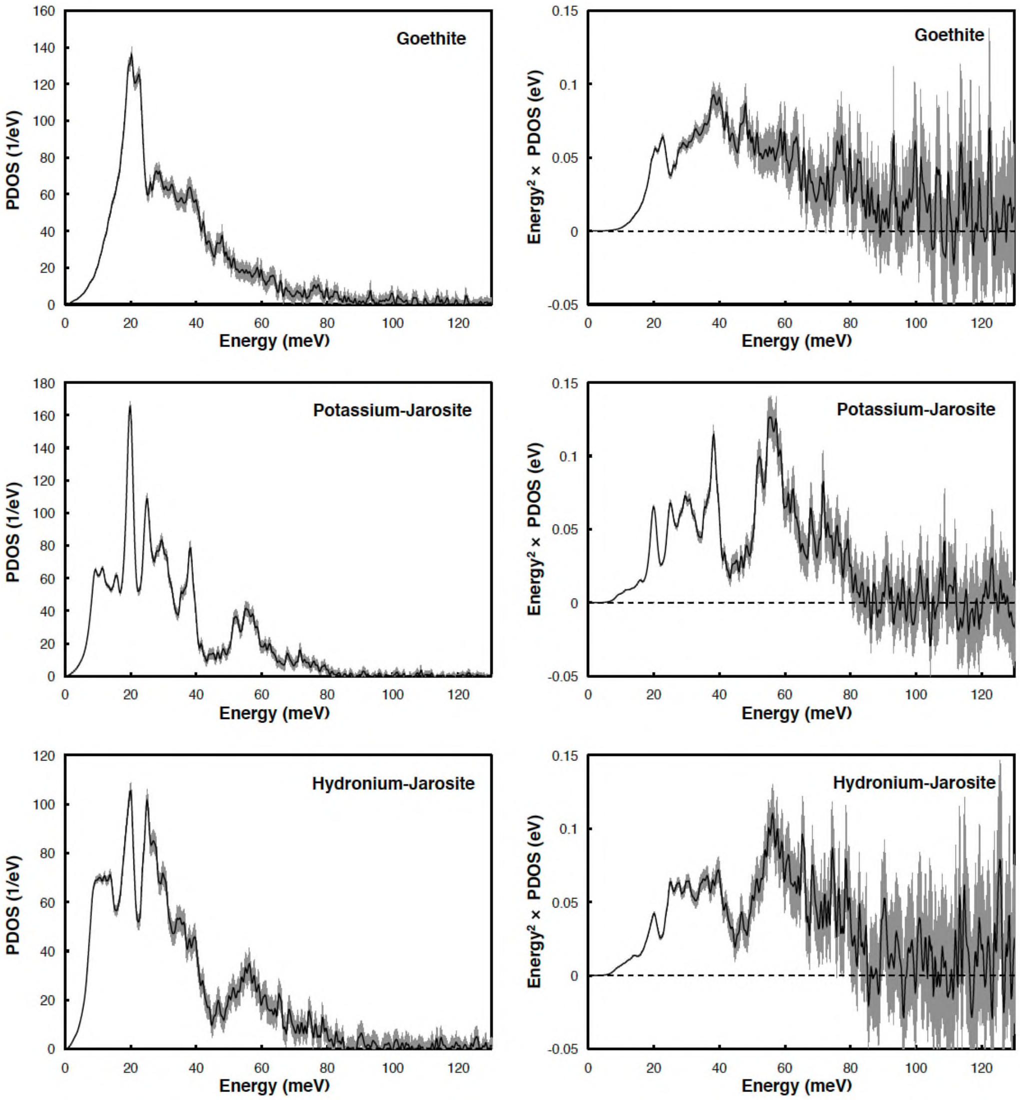
Difficulties with force constant measurements

$$\langle F \rangle \propto R_3^S$$



Difficulties with force constant measurements

$$\left\langle F \right\rangle \propto m_2^g$$

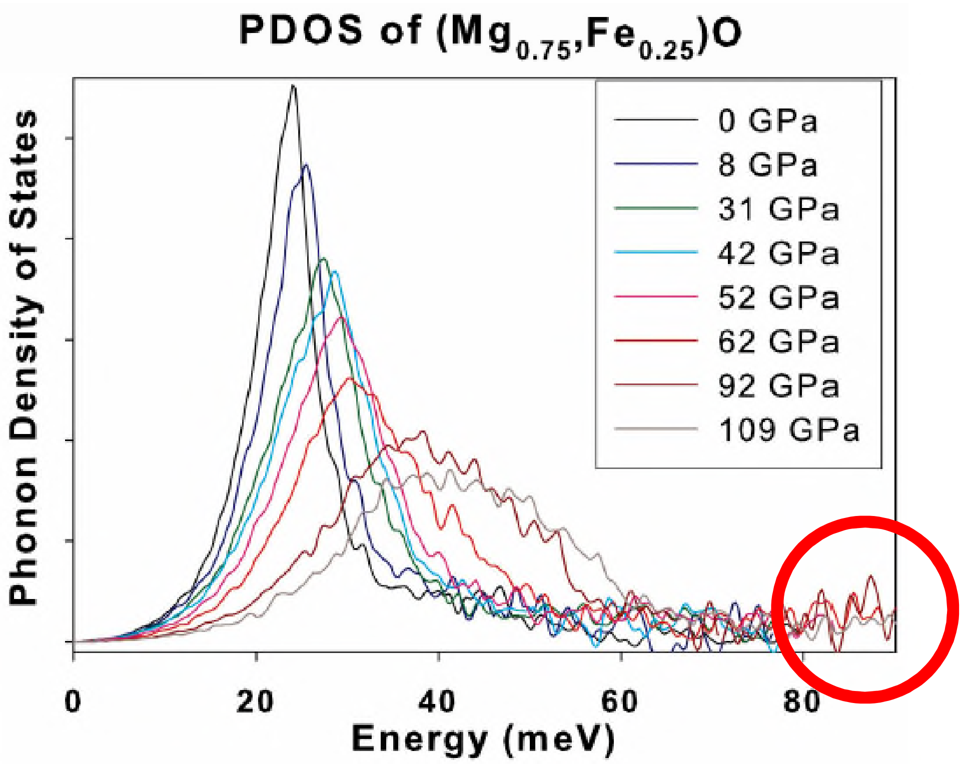


A word of caution with published data

Equilibrium Iron Isotope Fractionation at Core-Mantle Boundary Conditions

Veniamin B. Polyakov

13 FEBRUARY 2009 VOL 323 SCIENCE www.sciencemag.org

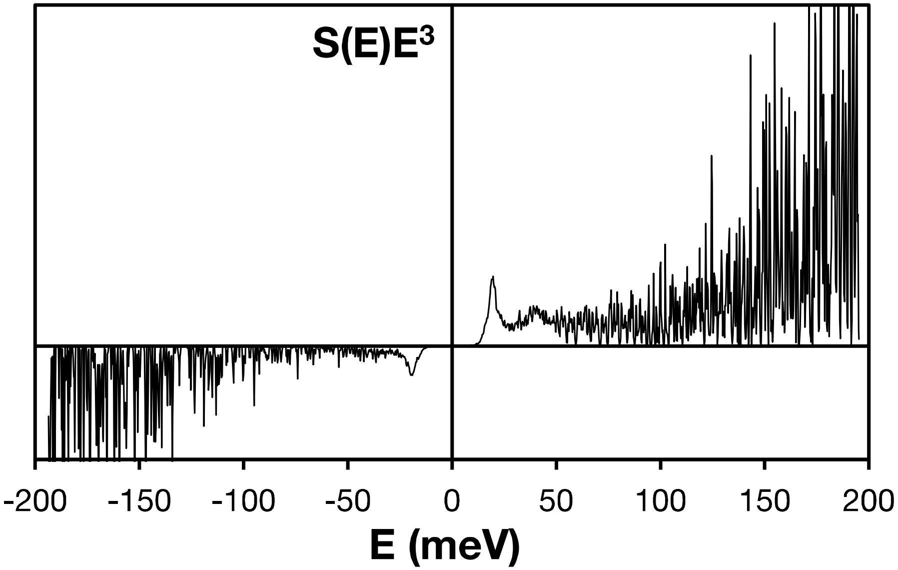


Lin et al. (2006)

Unaccounted baseline in NRIXS

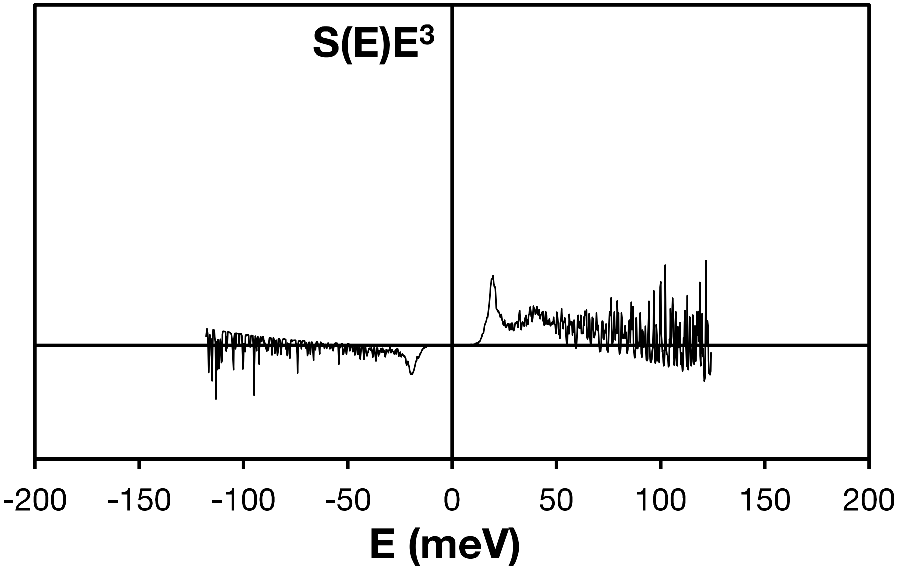
No baseline subtraction

⟨F⟩ = 968±128 N/m

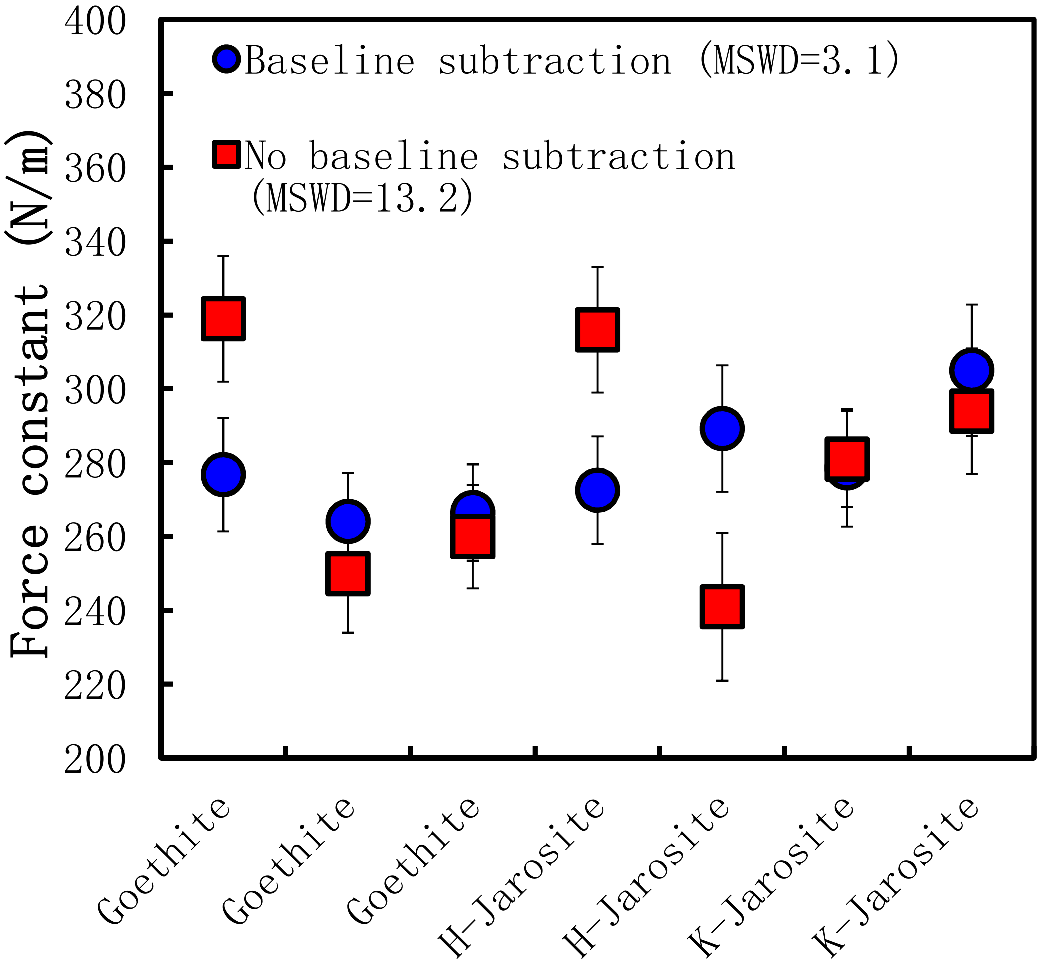


Baseline subtraction
with SciPhon

⟨F⟩ = 213±36 N/m



Baseline subtraction



Improves the session-to-session long term reproducibility

Error propagation in derived quantities

- Counting statistics

- Parameters of the baseline $(a \pm \sigma a)x+(b \pm \sigma b)$
- Zero energy bin
- Energy scaling
- Bin-to-bin energy variations

Hu et al. (2013); Dauphas et al. (2014)

Motivations for SciPhon

1. Have a GUI interface

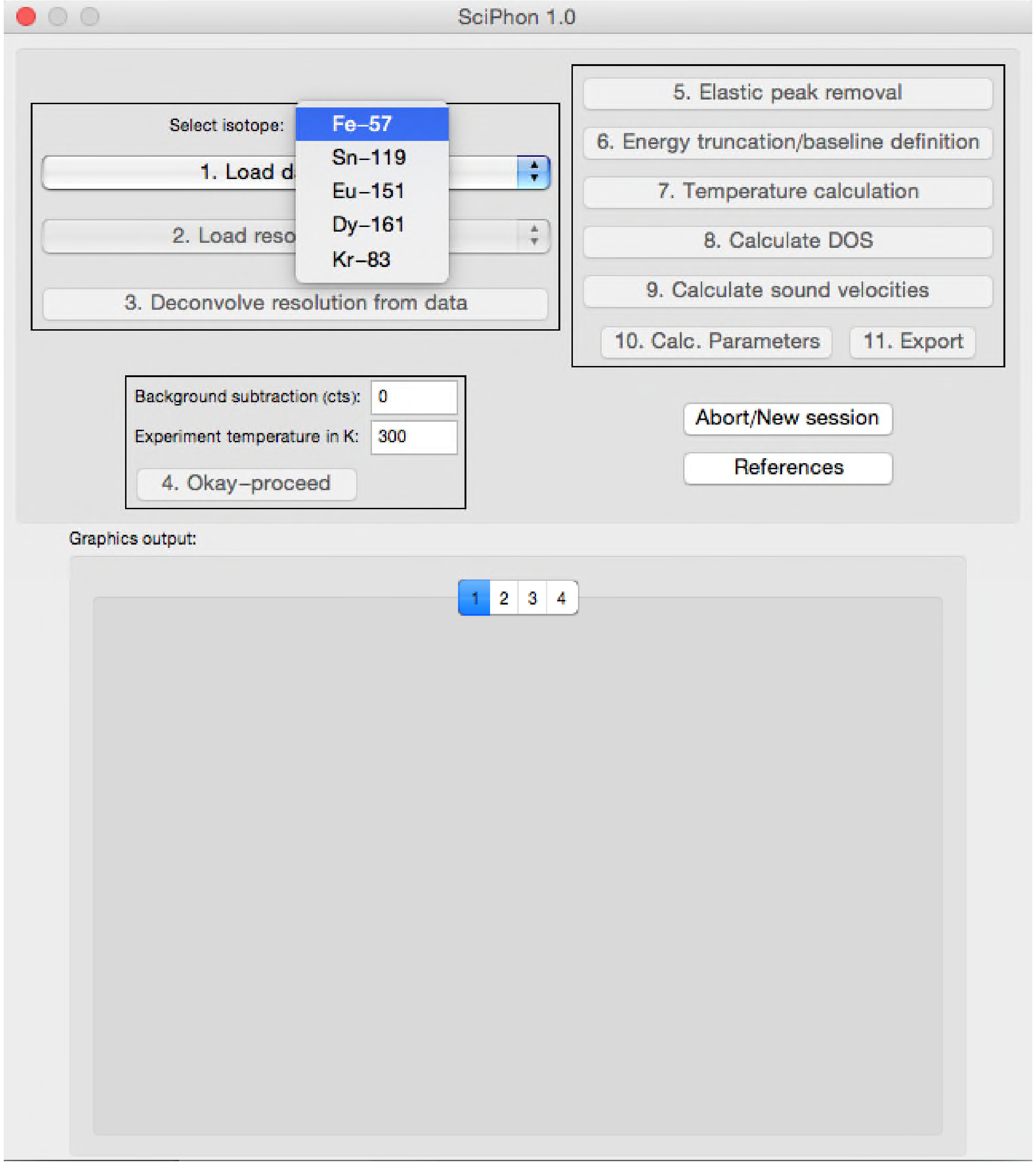
2. Streamline the baseline subtraction procedure

3. Propagate sources of uncertainties other than counting statistics

4. Output quantities directly usable in isotope geochemistry

SciPhon

Select a Mossbauer isotope (^{57}Fe default choice)

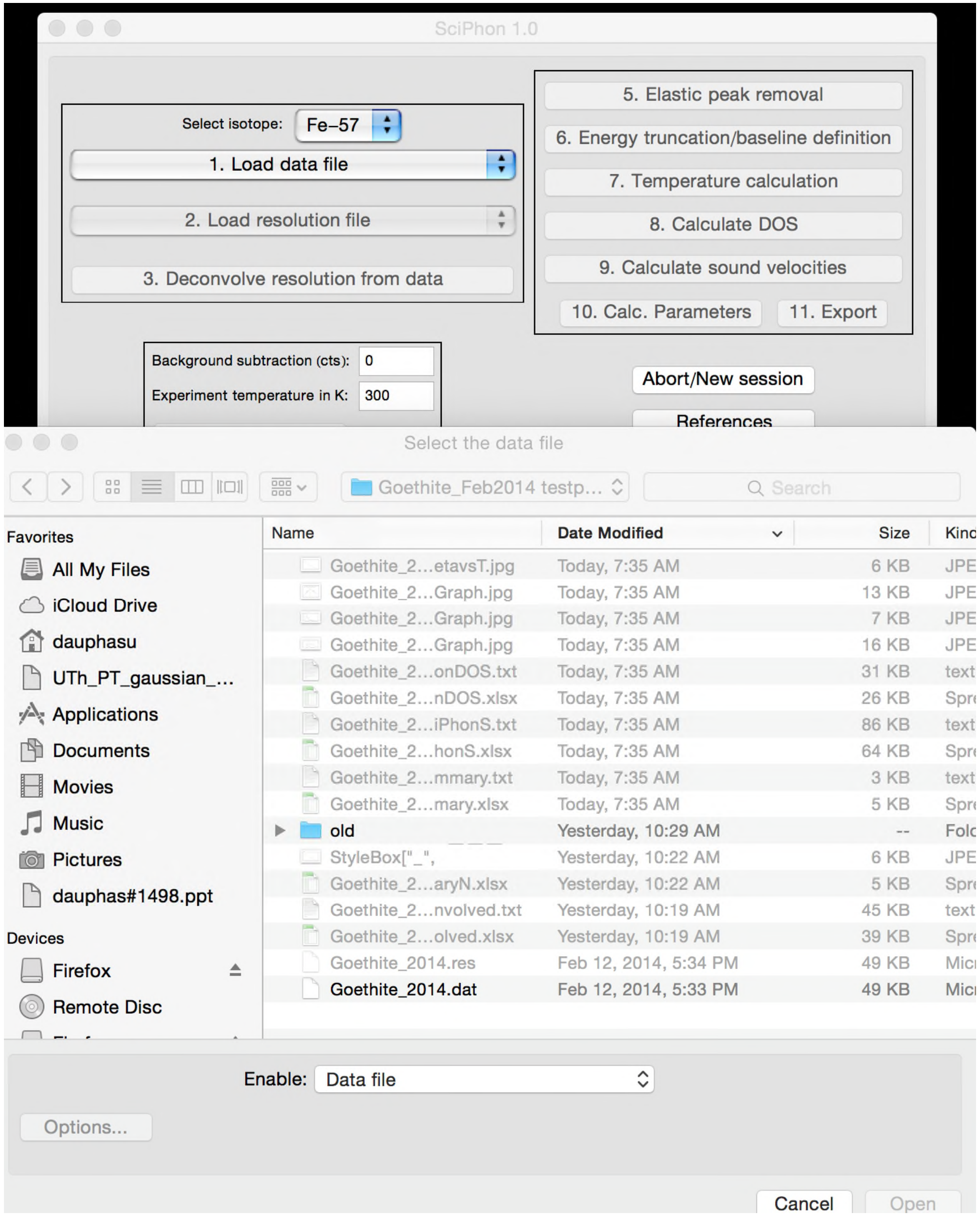


Select isotope: Fe–57

Background subtraction (cts): 0

Experiment temperature in K: 300

Load a “.dat” file (you need padd from Phoenix to make such a file)



Select isotope: Fe–57

Background subtraction (cts): 0

Experiment temperature in K: 300

Name	Date Modified	Size	Kin
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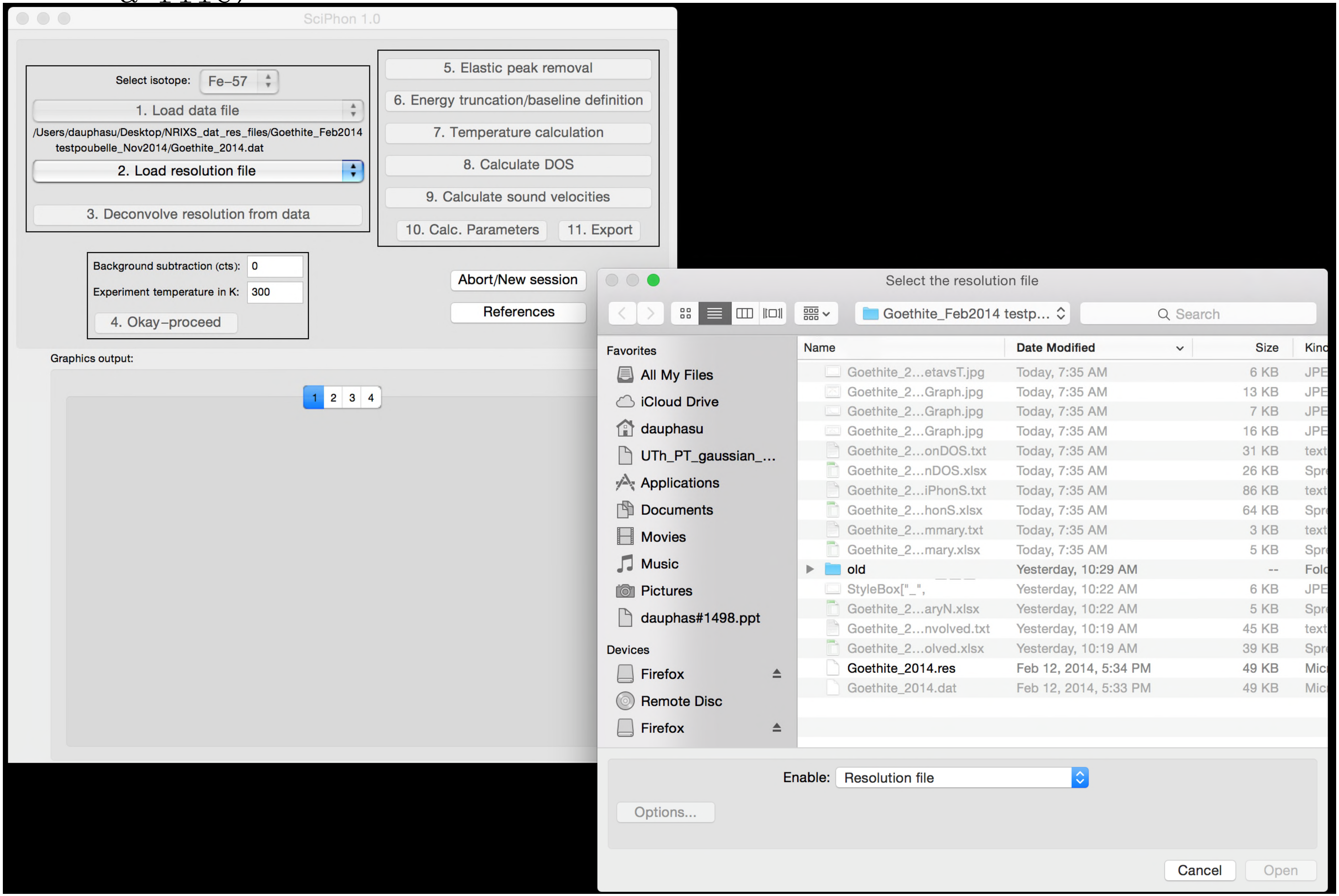
Goethite_2...Graph.jpg	Today, 7:35 AM	13 KB	JPE
Goethite_2...Graph.jpg	Today, 7:35 AM	7 KB	JPE
Goethite_2...Graph.jpg	Today, 7:35 AM	16 KB	JPE
Goethite_2...onDOS.txt	Today, 7:35 AM	31 KB	text
Goethite_2...nDOS.xlsx	Today, 7:35 AM	26 KB	Spr
Goethite_2...iPhonS.txt	Today, 7:35 AM	86 KB	text
Goethite_2...honS.xlsx	Today, 7:35 AM	64 KB	Spr
Goethite_2...mmary.txt	Today, 7:35 AM	3 KB	text
Goethite_2...mary.xlsx	Today, 7:35 AM	5 KB	Spr
old	Yesterday, 10:29 AM	--	Fol
StyleBox["_",	Yesterday, 10:22 AM	6 KB	JPE
Goethite_2...aryN.xlsx	Yesterday, 10:22 AM	5 KB	Spr
Goethite_2...nvolved.txt	Yesterday, 10:19 AM	45 KB	text
Goethite_2...olved.xlsx	Yesterday, 10:19 AM	39 KB	Spr
Goethite_2014.res	Feb 12, 2014, 5:34 PM	49 KB	Mic
Goethite_2014.dat	Feb 12, 2014, 5:33 PM	49 KB	Mic

Enable: Data file

Load a ".res" file (you need padd from Phoenix to make such a file)



/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.dat

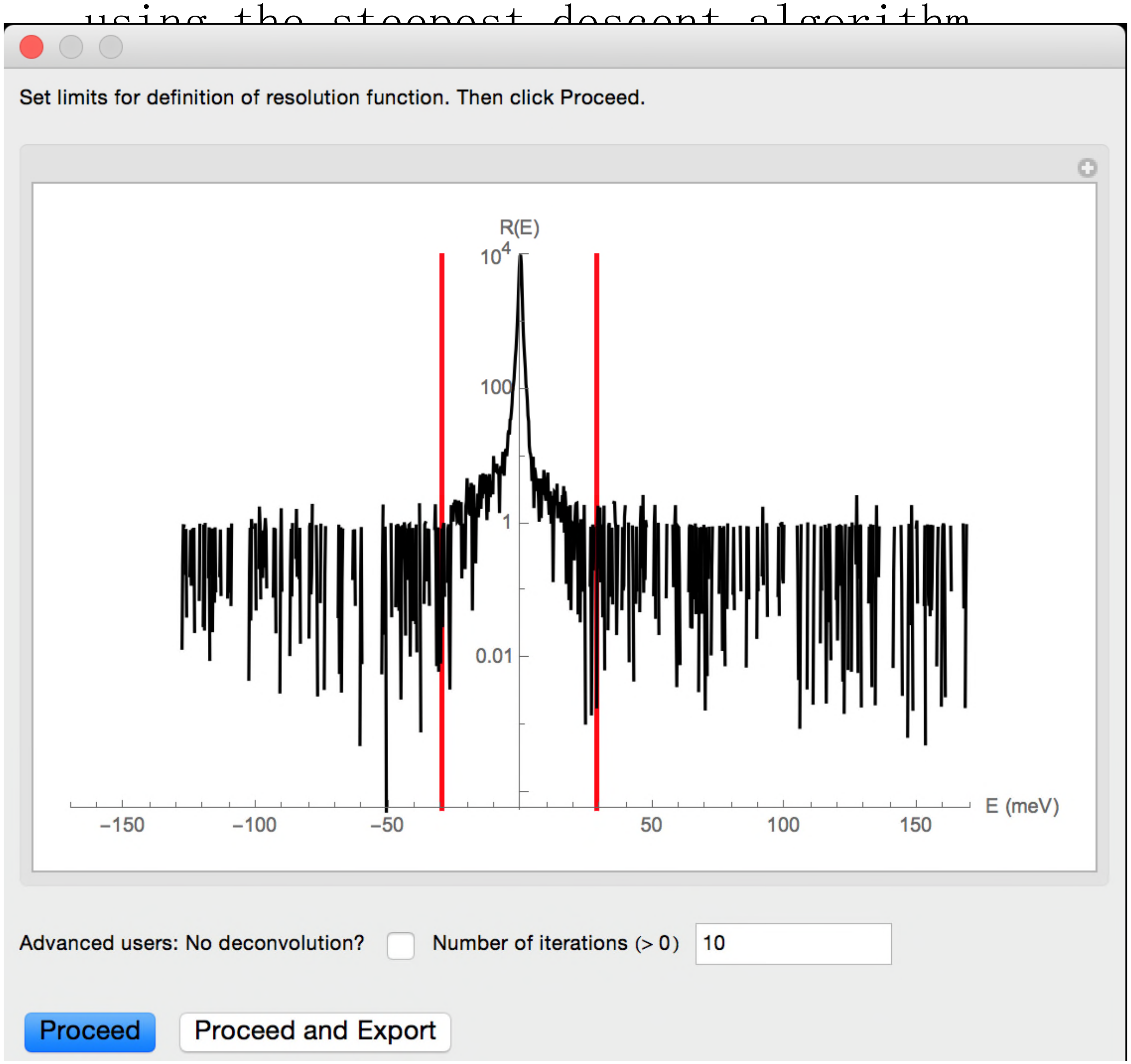
Background subtraction (cts): 0

Experiment temperature in K: 300

Name	Date Modified	Size	Kin
Goethite_2...etavsT.jpg	Today, 7:35 AM	6 KB	JPE
Goethite_2...Graph.jpg	Today, 7:35 AM	13 KB	JPE
Goethite_2...Graph.jpg	Today, 7:35 AM	7 KB	JPE
Goethite_2...Graph.jpg	Today, 7:35 AM	16 KB	JPE
Goethite_2...onDOS.txt	Today, 7:35 AM	31 KB	text
Goethite_2...nDOS.xlsx	Today, 7:35 AM	26 KB	Spr
Goethite_2...iPhonS.txt	Today, 7:35 AM	86 KB	text
Goethite_2...honS.xlsx	Today, 7:35 AM	64 KB	Spr
Goethite_2...mmary.txt	Today, 7:35 AM	3 KB	text
Goethite_2...mary.xlsx	Today, 7:35 AM	5 KB	Spr
old	Yesterday, 10:29 AM	--	Fold
StyleBox["_",	Yesterday, 10:22 AM	6 KB	JPE
Goethite_2...aryN.xlsx	Yesterday, 10:22 AM	5 KB	Spr
Goethite_2...nvolved.txt	Yesterday, 10:19 AM	45 KB	text
Goethite_2...olved.xlsx	Yesterday, 10:19 AM	39 KB	Spr
Goethite_2014.res	Feb 12, 2014, 5:34 PM	49 KB	Mic
Goethite_2014.dat	Feb 12, 2014, 5:33 PM	49 KB	Mic

Enable: Resolution file

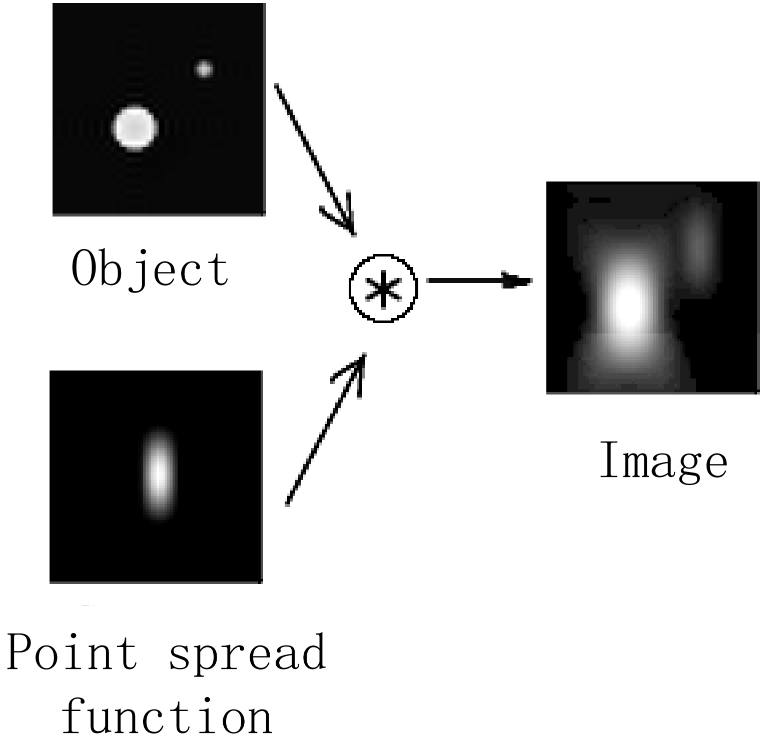
Deconvolution of the resolution from the data using the steepest descent algorithm



Set limits for definition of resolution function. Then click Proceed.

Advanced users: No deconvolution? ☐ Number of iterations (> 0) 10

Deconvolution



Object

Point spread function

Image

Deconvolution

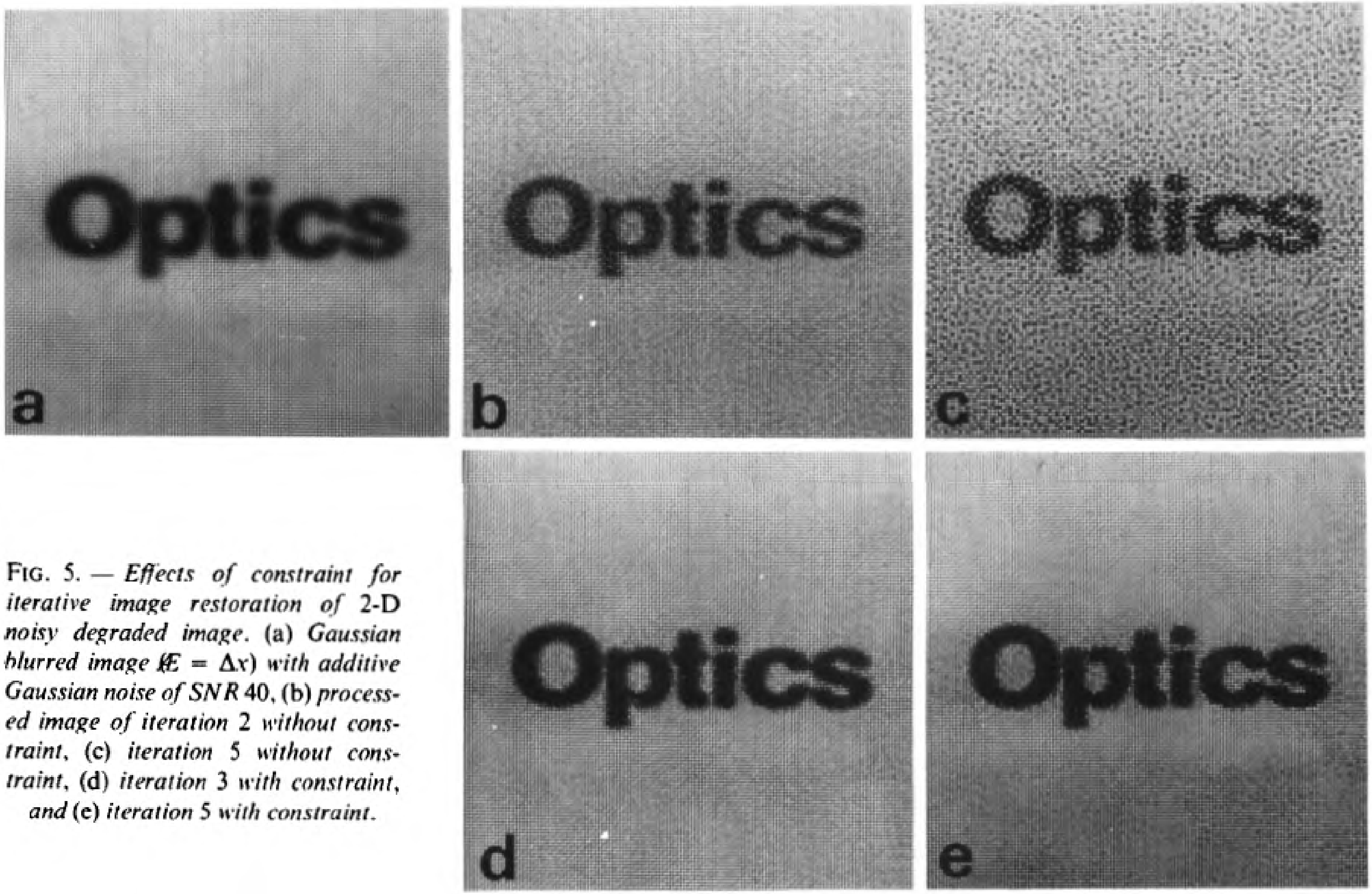
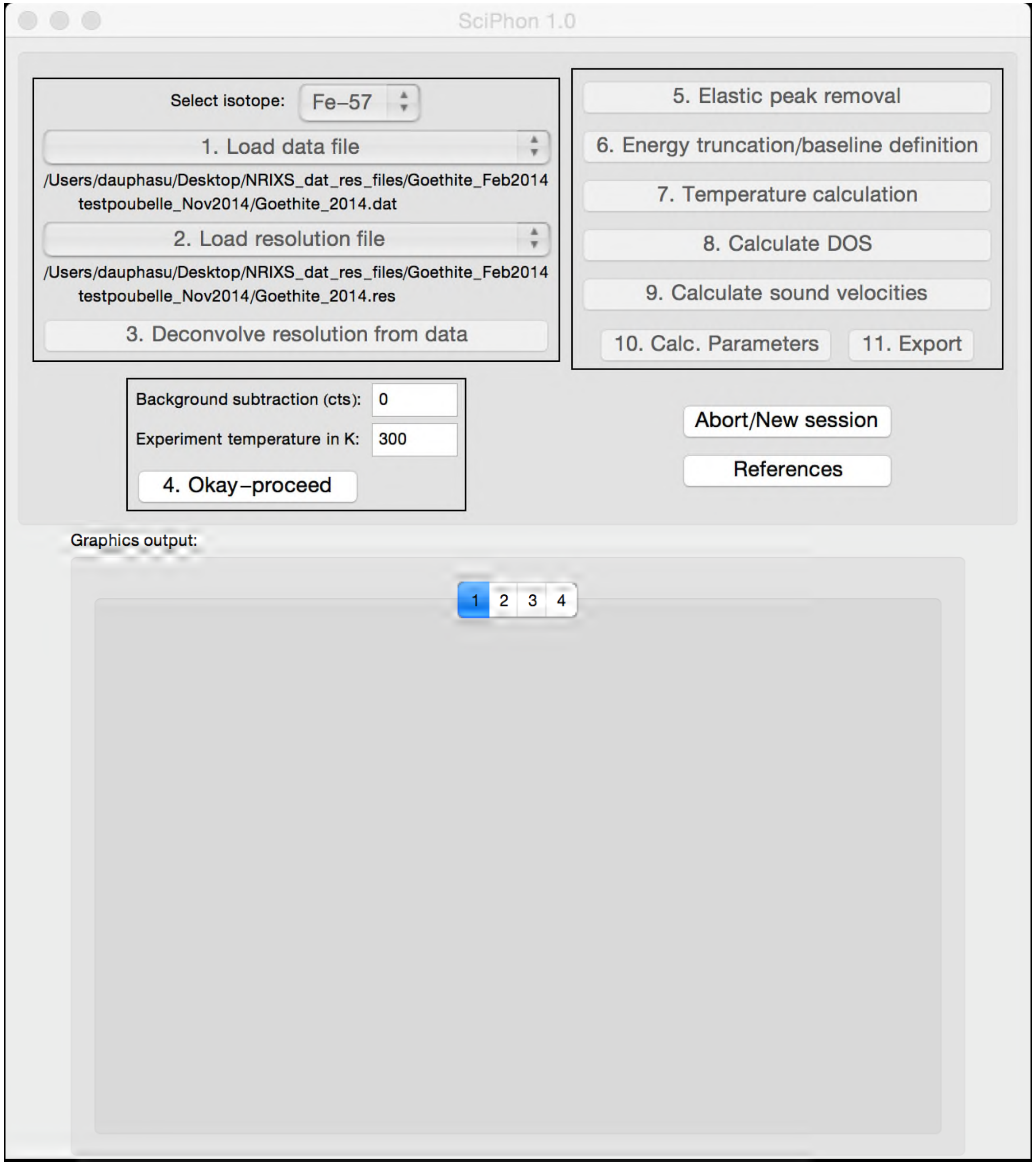


FIG. 5. — *Effects of constraint for iterative image restoration of* 2-D *noisy degraded image.* (a) *Gaussian blurred image* (Æ = Δx) *with additive Gaussian noise of SNR* 40, (b) *processed image of iteration* 2 *without constraint,* (c) *iteration* 5 *without constraint,* (d) *iteration* 3 *with constraint, and* (e) *iteration* 5 *with constraint.*

In the steepest descent algorithm, the restoration vector is manipulated so as to only return positive values and reduce oscillations (Ichioka et al., 1981)

Noise amplification can be limited by terminating the algorithm after a finite number of iterations

Input the experiment temperature and background



Select isotope: Fe–57

/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.dat

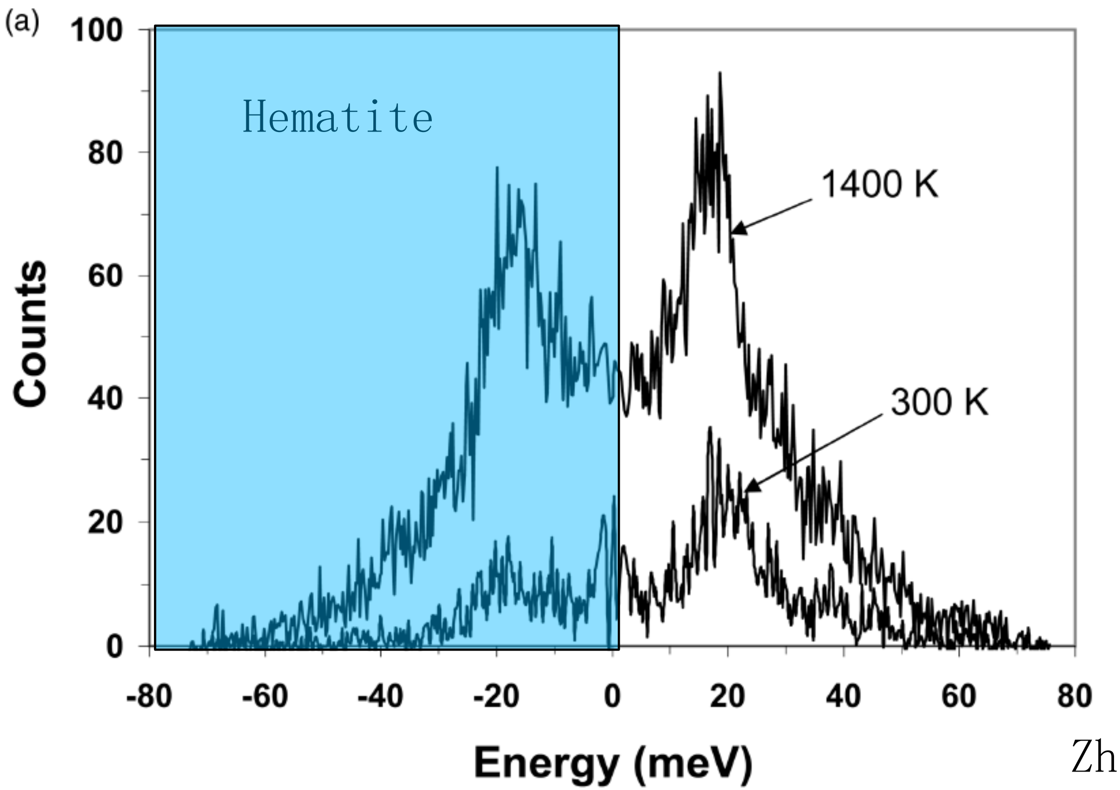
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.res

Background subtraction (cts): 0

Experiment temperature in K: 300

Detailed balance

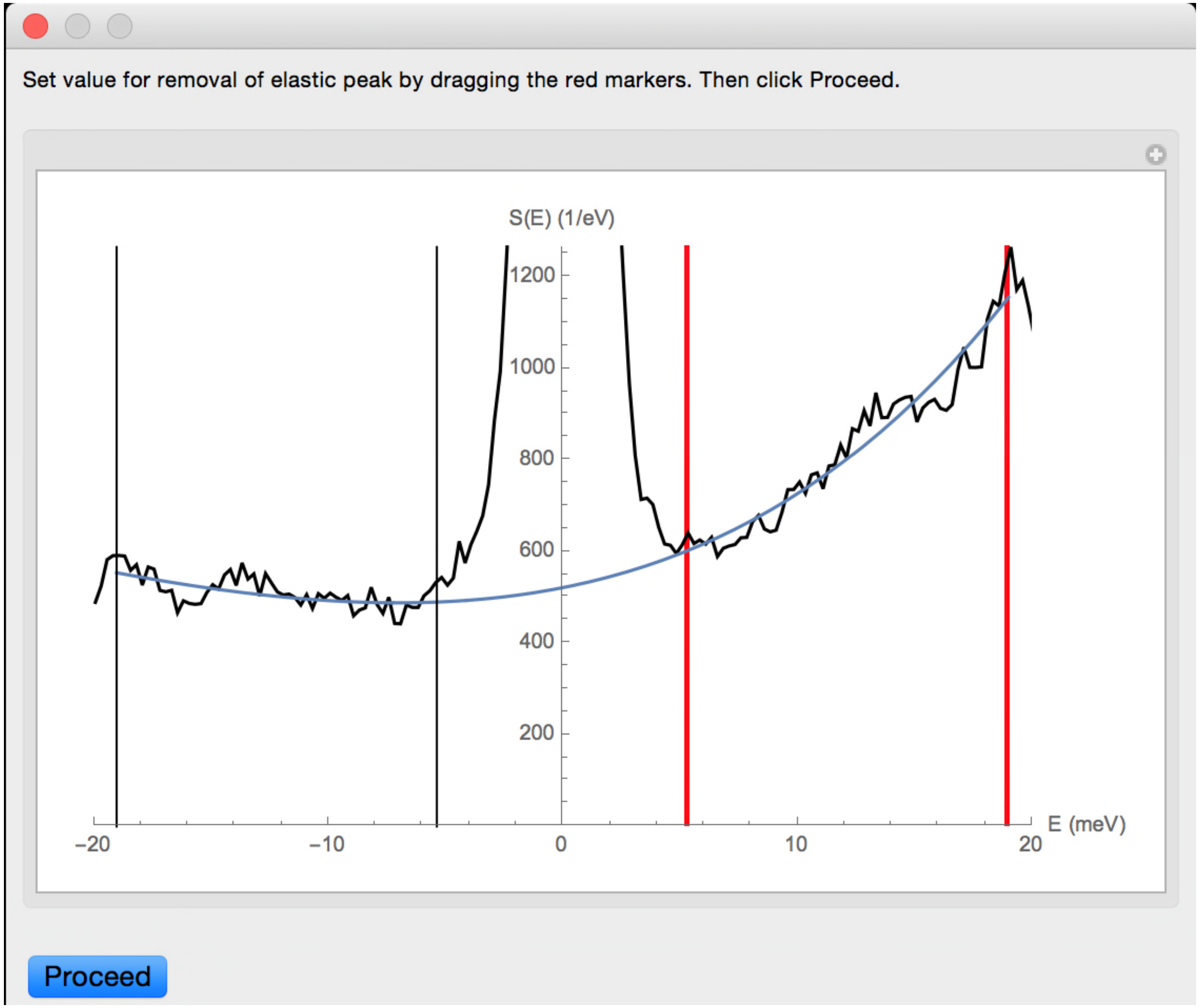
$$\frac{I(E)}{I(-E)} = e^{E/kT}$$



Zhao et al. (2004)

The phonon annihilation part is used. It added to the phonon creation part by applying the proper weights and using the experimental

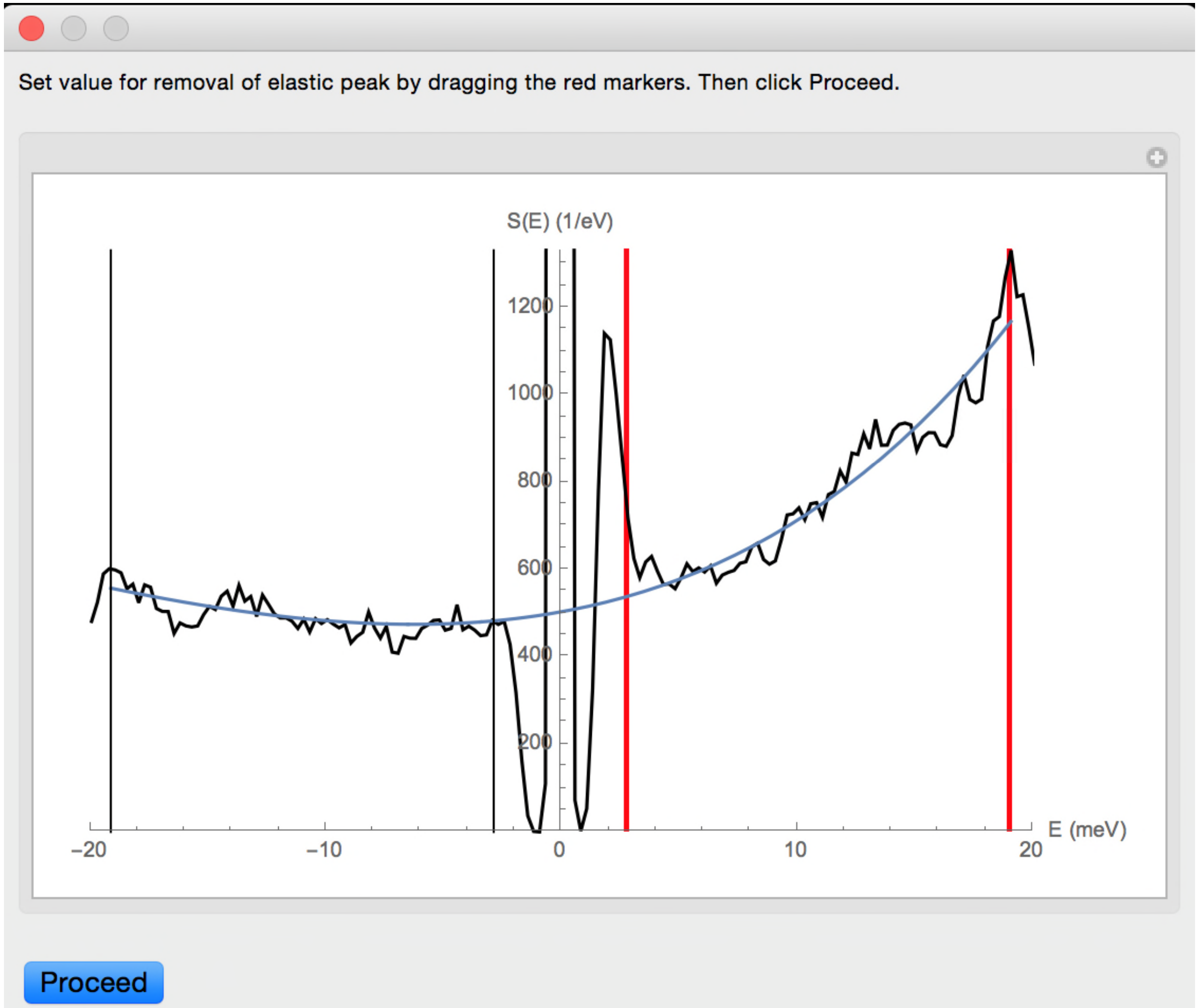
Elastic peak removal



Set value for removal of elastic peak by dragging the red markers. Then click Proceed.

No peak deconvolution

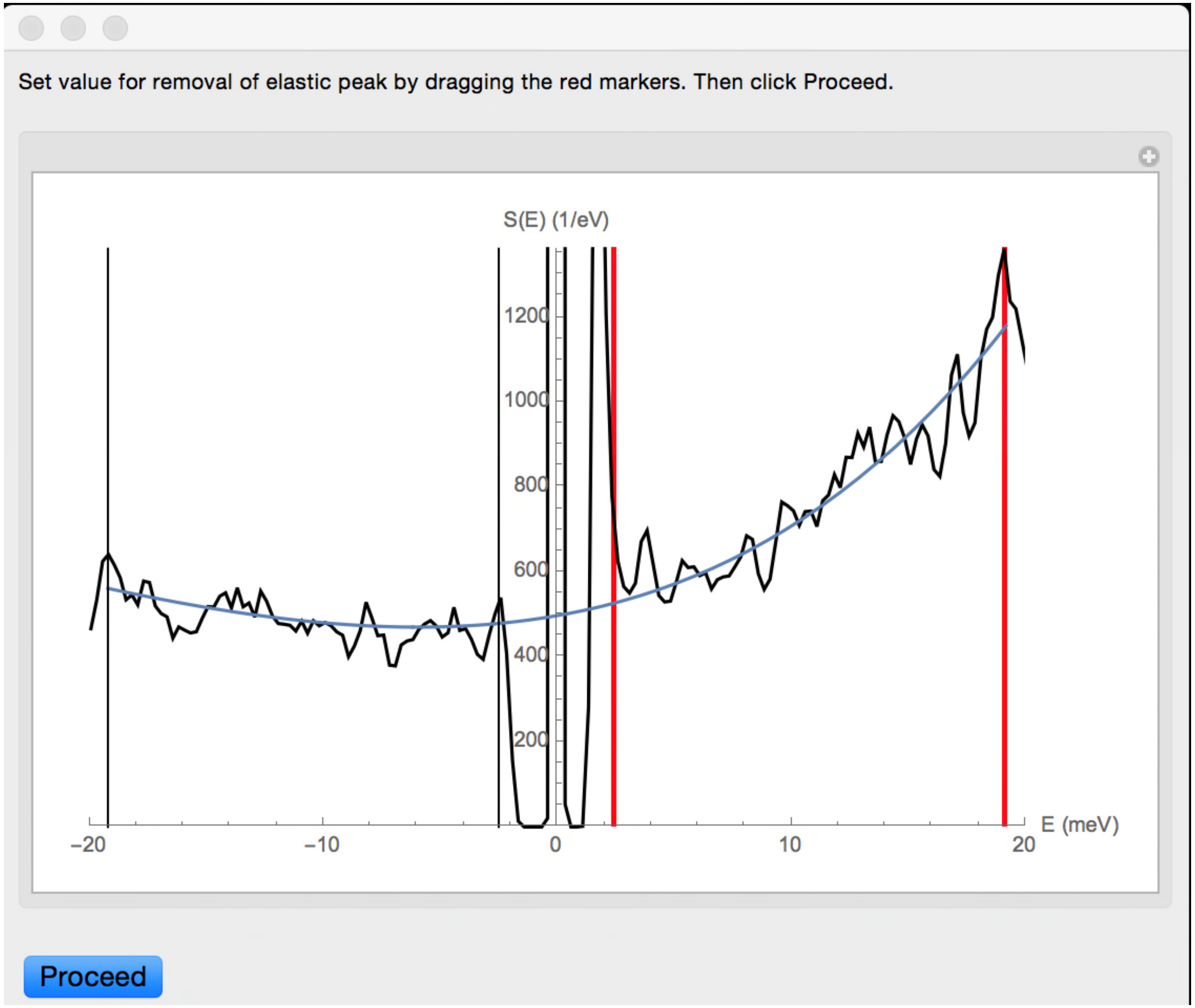
Elastic peak removal



Set value for removal of elastic peak by dragging the red markers. Then click Proceed.

10 iterations

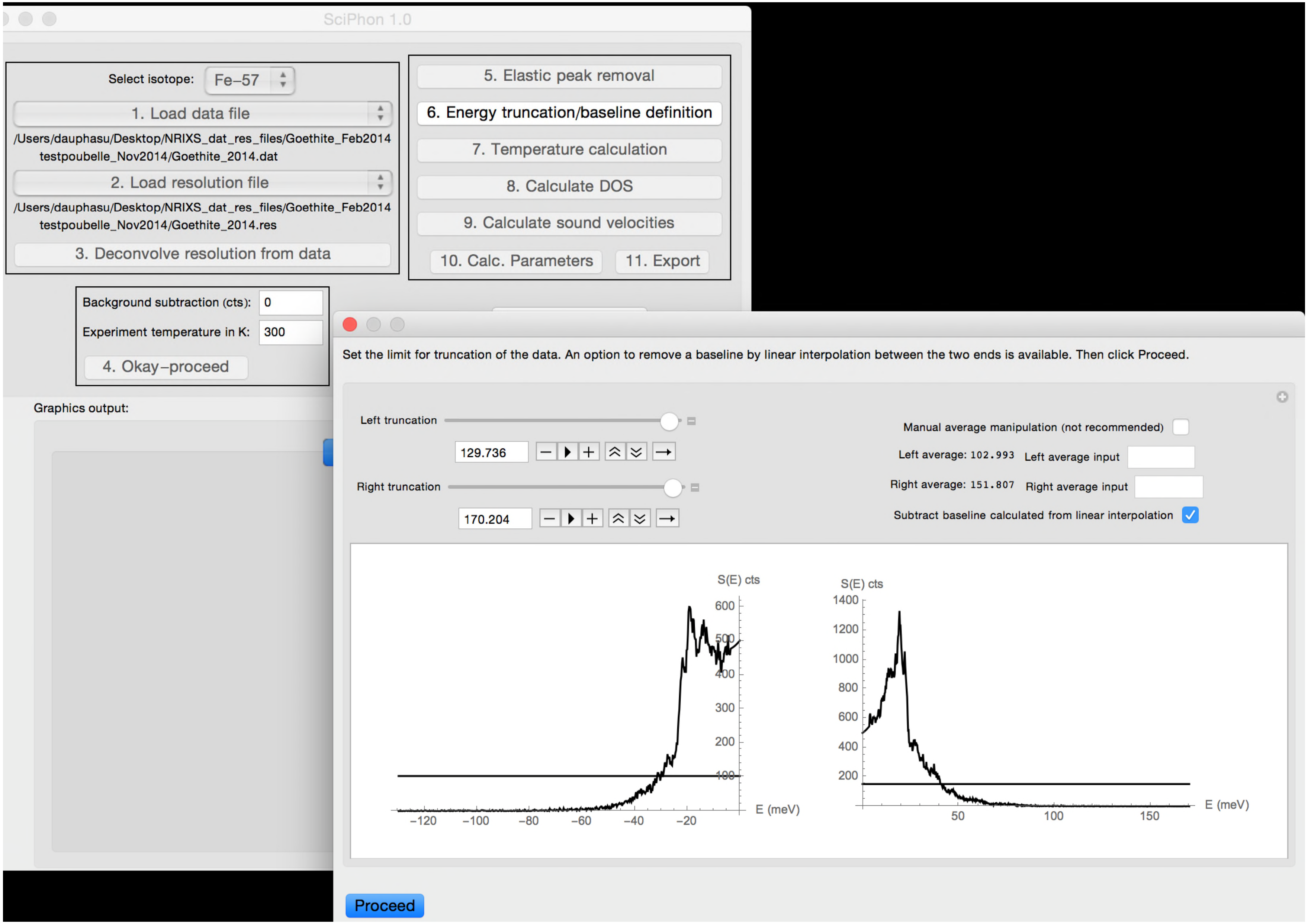
Elastic peak removal



Set value for removal of elastic peak by dragging the red markers. Then click Proceed.

1000 iterations

Truncation and baseline definition



Select isotope: Fe–57

/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.dat

/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.res

Background subtraction (cts): 0

Experiment temperature in K: 300

Set the limit for truncation of the data. An option to remove a baseline by linear interpolation between the two ends is available. Then click Proceed.

Left truncation: 129.736

Right truncation: 170.204

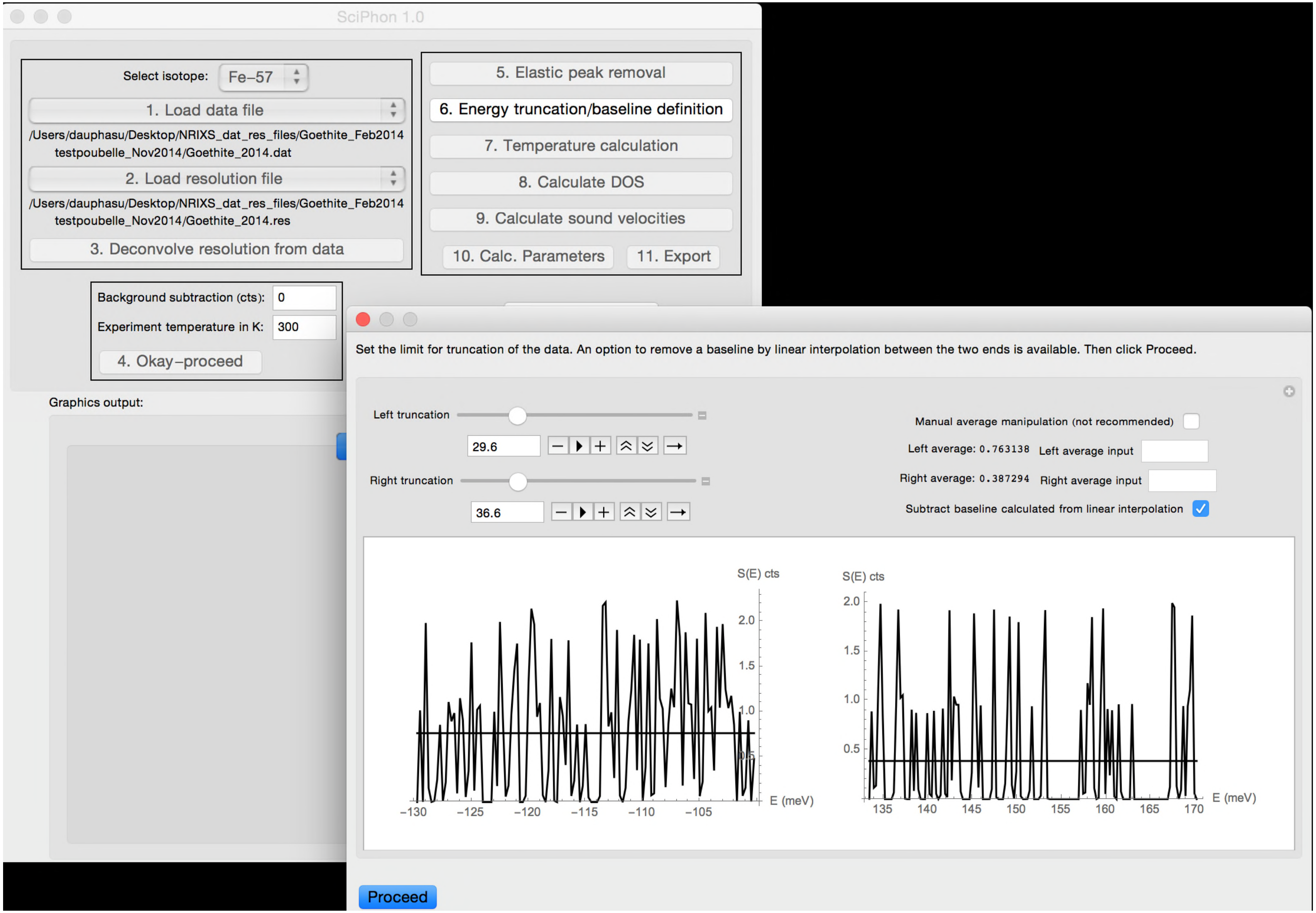
Manual average manipulation (not recommended) ☐

Left average: `102.993` Left average input

Right average: `151.807` Right average input

Subtract baseline calculated from linear interpolation ☑

Truncation and baseline definition



Select isotope: Fe–57

/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.dat

/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.res

Background subtraction (cts): 0

Experiment temperature in K: 300

Set the limit for truncation of the data. An option to remove a baseline by linear interpolation between the two ends is available. Then click Proceed.

Left truncation: 29.6

Right truncation: 36.6

Manual average manipulation (not recommended) ☐

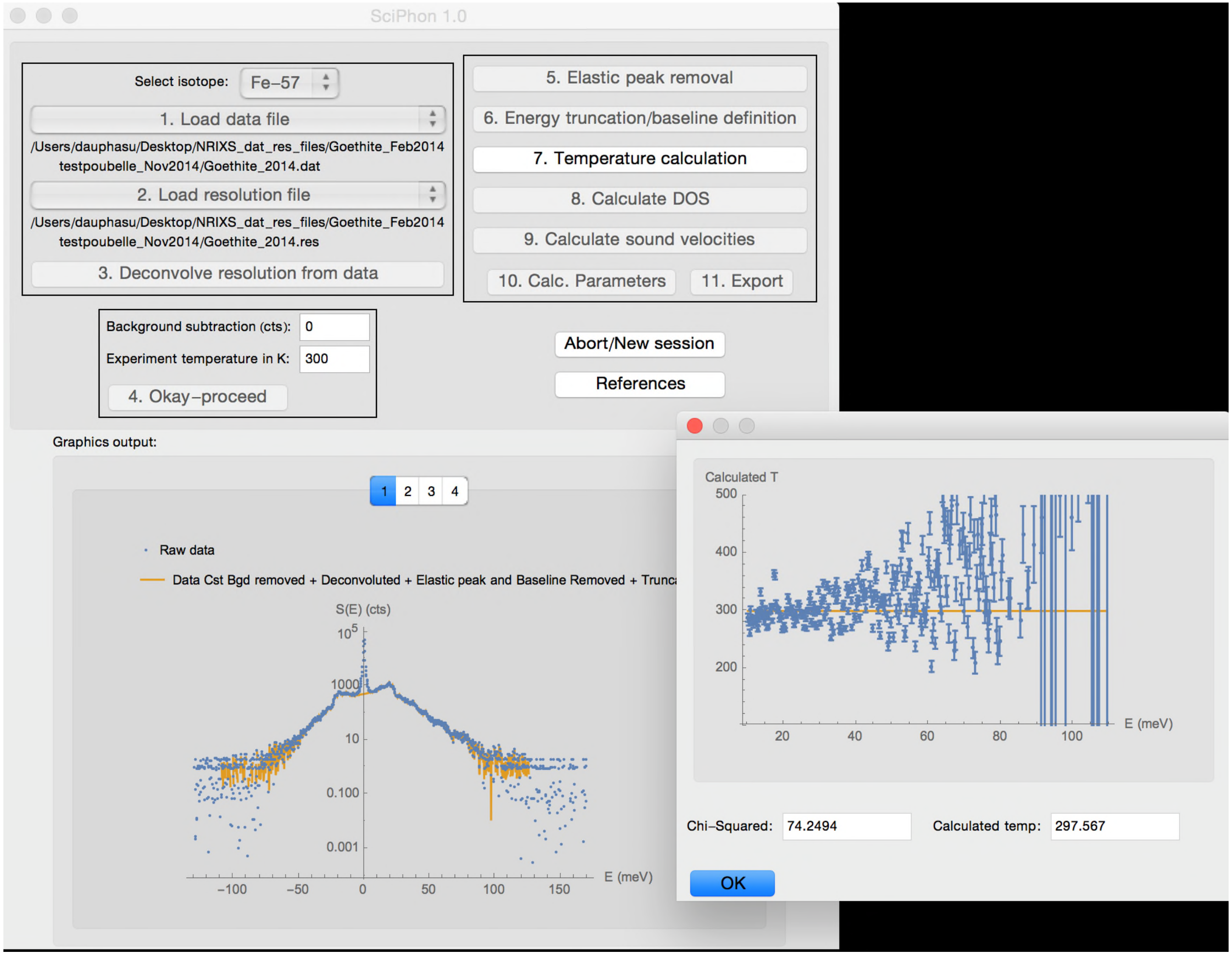
Left average: 0.763138 Left average input

Right average: 0.387294 Right average input

Subtract baseline calculated from linear interpolation ☑

Temperature determination

$$\frac{I(E)}{I(-E)} = e^{E/kT}$$



Select isotope: Fe–57

/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.dat

/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.res

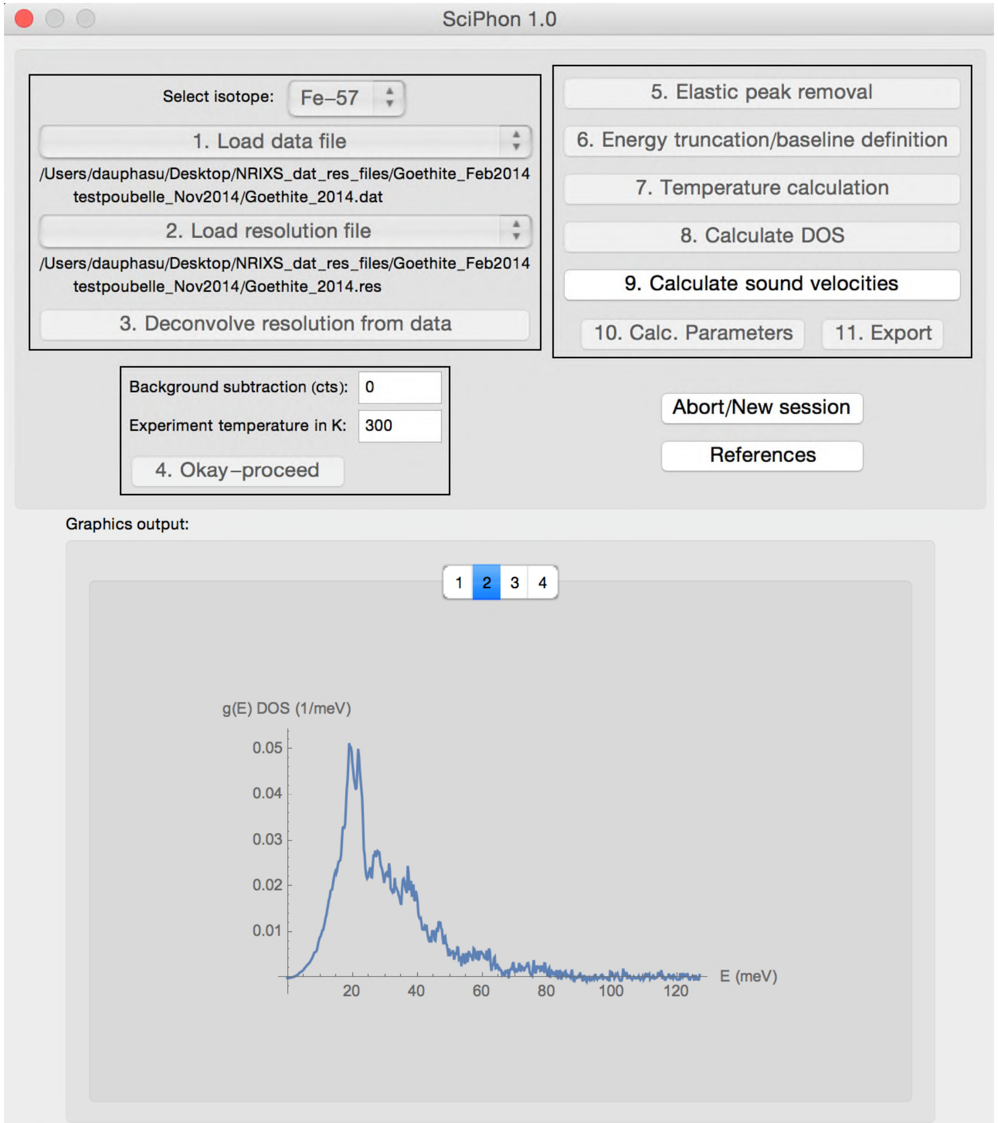
Background subtraction (cts): 0

Experiment temperature in K: 300

Chi–Squared: 74.2494

Calculated temp: 297.567

DOS calculation



SciPhon 1.0

Select isotope: Fe–57

/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.dat

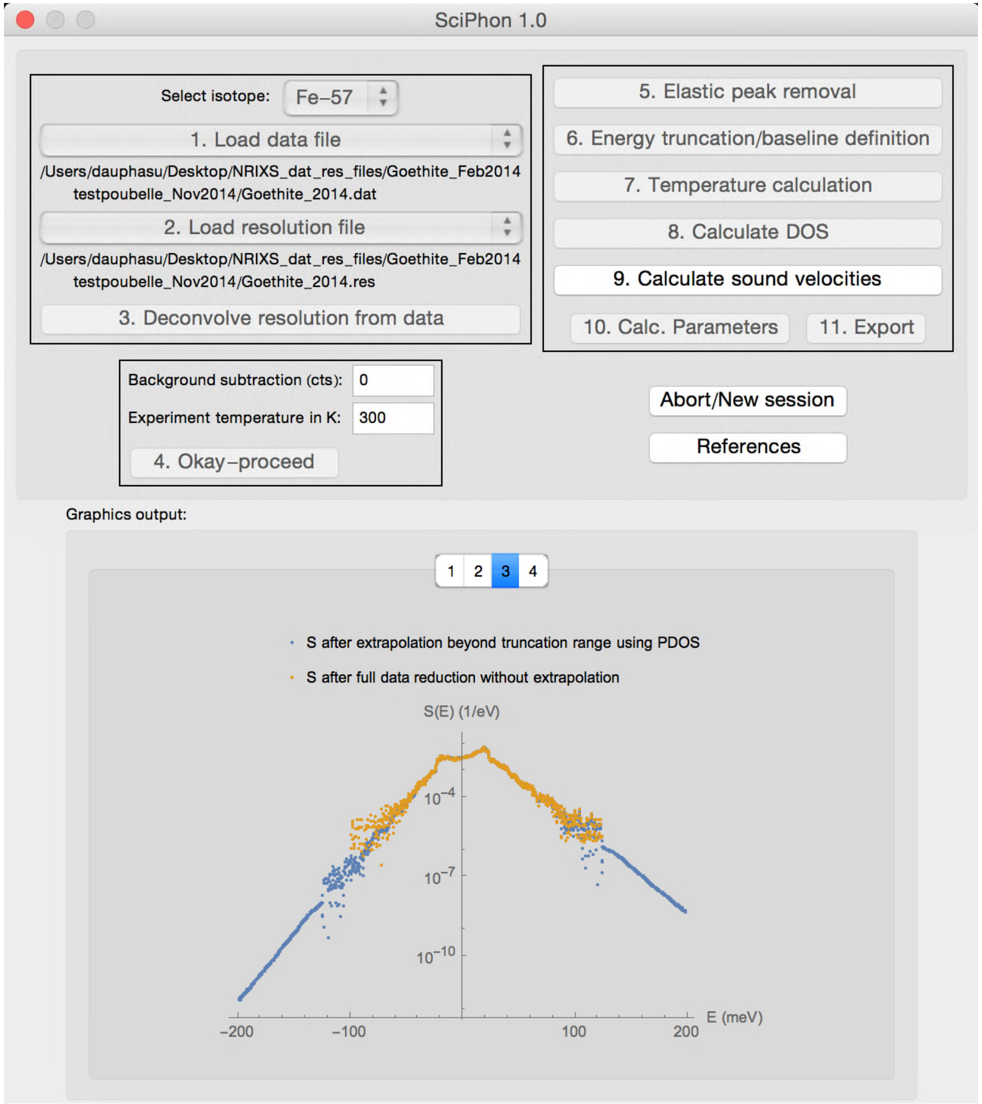
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.res

Background subtraction (cts): 0

Experiment temperature in K: 300

Graphics output:

Extrapolation beyond the truncation range using the DOS



Select isotope: Fe–57

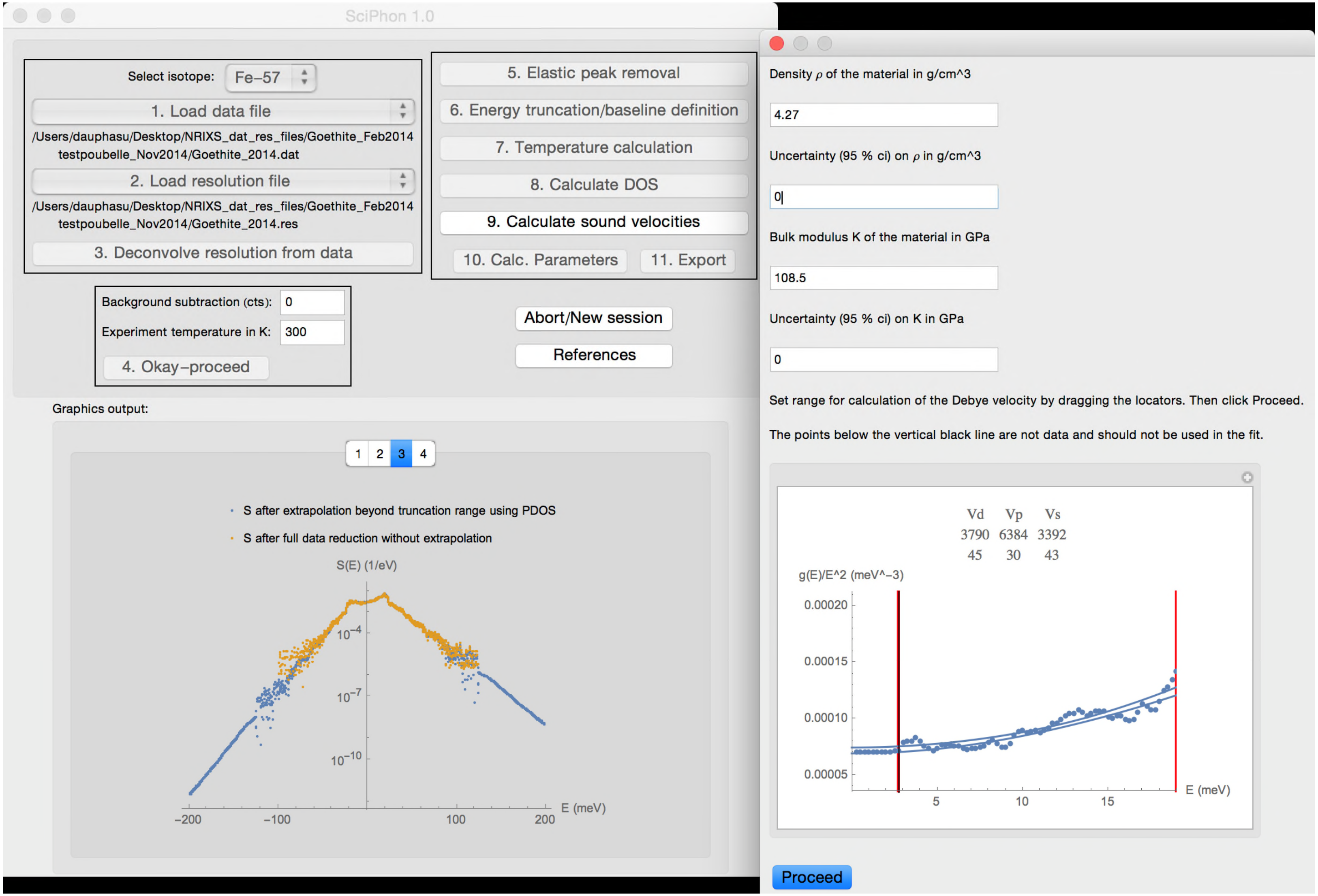
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014
testpoubelle_Nov2014/Goethite_2014.dat

/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014
testpoubelle_Nov2014/Goethite_2014.res

Background subtraction (cts): 0

Experiment temperature in K: 300

Calculate sound velocities



Select isotope: Fe−57

/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.dat

/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.res

Background subtraction (cts): 0

Experiment temperature in K: 300

Density ρ of the material in g/cm^3

4.27

Uncertainty (95 % ci) on ρ in g/cm^3

0

Bulk modulus K of the material in GPa

108.5

Uncertainty (95 % ci) on K in GPa

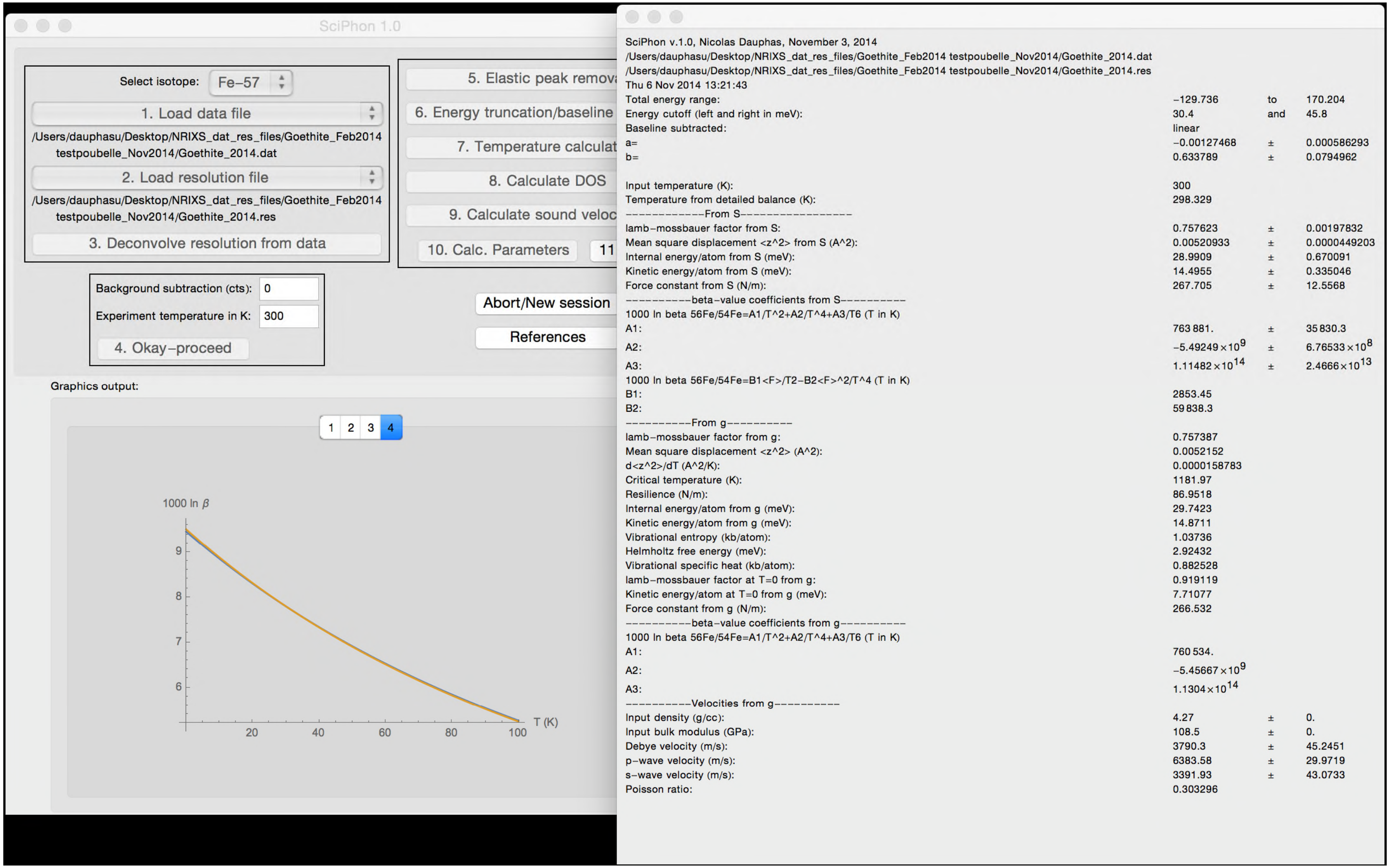
0

Set range for calculation of the Debye velocity by dragging the locators. Then click Proceed.

The points below the vertical black line are not data and should not be used in the fit.

Vd	Vp	Vs
3790	6384	3392
45	30	43

Calculated parameters



Select isotope: Fe–57

/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.dat

/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.res

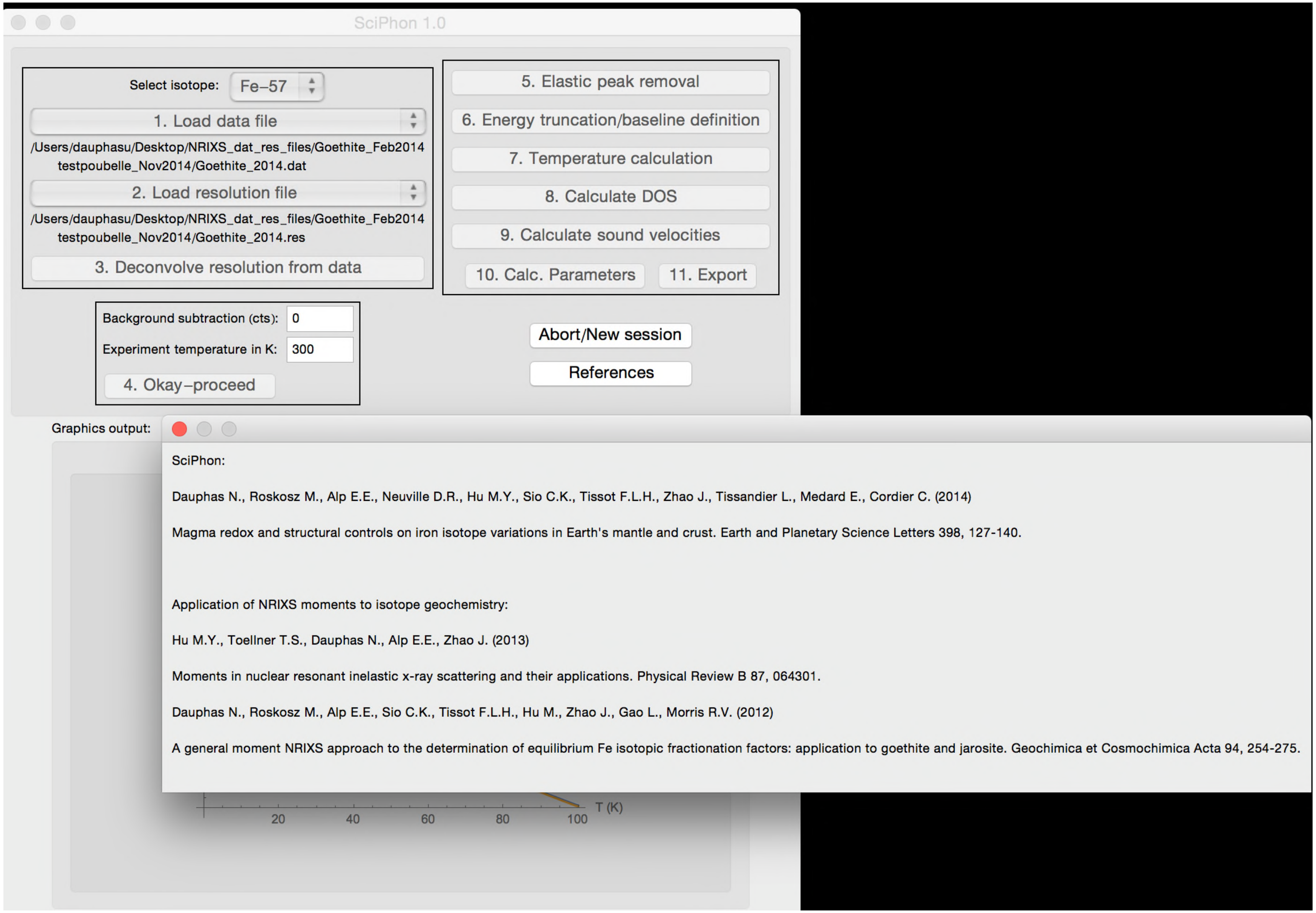
Background subtraction (cts): 0

Experiment temperature in K: 300

```
SciPhon v.1.0, Nicolas Dauphas, November 3, 2014
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.dat
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.res
Thu 6 Nov 2014 13:21:43
Total energy range:                                    −129.736        to     170.204
Energy cutoff (left and right in meV):                 30.4            and    45.8
Baseline subtracted:                                   linear
a=                                                     −0.00127468     ±      0.000586293
b=                                                     0.633789        ±      0.0794962

Input temperature (K):                                 300
Temperature from detailed balance (K):                 298.329
−−−−−−−−−−−−From S−−−−−−−−−−−−−−−−−
lamb−mossbauer factor from S:                          0.757623        ±      0.00197832
Mean square displacement <z^2> from S (A^2):           0.00520933      ±      0.0000449203
Internal energy/atom from S (meV):                     28.9909         ±      0.670091
Kinetic energy/atom from S (meV):                      14.4955         ±      0.335046
Force constant from S (N/m):                           267.705         ±      12.5568
−−−−−−−−−−beta−value coefficients from S−−−−−−−−−−
1000 ln beta 56Fe/54Fe=A1/T^2+A2/T^4+A3/T6 (T in K)
A1:                                                    763 881.        ±      35 830.3
A2:                                                    −5.49249×10^9   ±      6.76533×10^8
A3:                                                    1.11482×10^14   ±      2.4666×10^13
1000 ln beta 56Fe/54Fe=B1<F>/T2−B2<F>^2/T^4 (T in K)
B1:                                                    2853.45
B2:                                                    59 838.3
−−−−−−−−−−From g−−−−−−−−−−
lamb−mossbauer factor from g:                          0.757387
Mean square displacement <z^2> (A^2):                  0.0052152
d<z^2>/dT (A^2/K):                                     0.0000158783
Critical temperature (K):                              1181.97
Resilience (N/m):                                      86.9518
Internal energy/atom from g (meV):                     29.7423
Kinetic energy/atom from g (meV):                      14.8711
Vibrational entropy (kb/atom):                         1.03736
Helmholtz free energy (meV):                           2.92432
Vibrational specific heat (kb/atom):                   0.882528
lamb−mossbauer factor at T=0 from g:                   0.919119
Kinetic energy/atom at T=0 from g (meV):               7.71077
Force constant from g (N/m):                           266.532
−−−−−−−−−−beta−value coefficients from g−−−−−−−−−−
1000 ln beta 56Fe/54Fe=A1/T^2+A2/T^4+A3/T6 (T in K)
A1:                                                    760 534.
A2:                                                    −5.45667×10^9
A3:                                                    1.1304×10^14
−−−−−−−−−−Velocities from g−−−−−−−−−−
Input density (g/cc):                                  4.27            ±      0.
Input bulk modulus (GPa):                              108.5           ±      0.
Debye velocity (m/s):                                  3790.3          ±      45.2451
p−wave velocity (m/s):                                 6383.58         ±      29.9719
s−wave velocity (m/s):                                 3391.93         ±      43.0733
Poisson ratio:                                         0.303296
```

References



Select isotope: Fe–57

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/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014 testpoubelle_Nov2014/Goethite_2014.res

Background subtraction (cts): 0

Experiment temperature in K: 300

SciPhon:

Dauphas N., Roskosz M., Alp E.E., Neuville D.R., Hu M.Y., Sio C.K., Tissot F.L.H., Zhao J., Tissandier L., Medard E., Cordier C. (2014)

Magma redox and structural controls on iron isotope variations in Earth's mantle and crust. Earth and Planetary Science Letters 398, 127-140.

Application of NRIXS moments to isotope geochemistry:

Hu M.Y., Toellner T.S., Dauphas N., Alp E.E., Zhao J. (2013)

Moments in nuclear resonant inelastic x-ray scattering and their applications. Physical Review B 87, 064301.

Dauphas N., Roskosz M., Alp E.E., Sio C.K., Tissot F.L.H., Hu M., Zhao J., Gao L., Morris R.V. (2012)

A general moment NRIXS approach to the determination of equilibrium Fe isotopic fractionation factors: application to goethite and jarosite. Geochimica et Cosmochimica Acta 94, 254-275.

Conclusions

NRIXS is a powerful tool in isotope geochemistry

Beware of the baseline in NRIXS

Use SciPhon and give us some feedback

SciPhon

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