

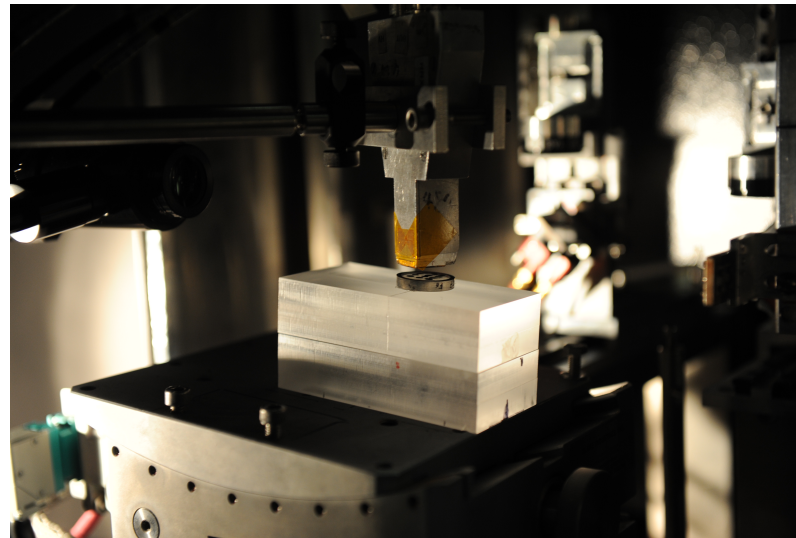


ORIGINS
LAB



Introduction to isotope fractionation and SciPhon

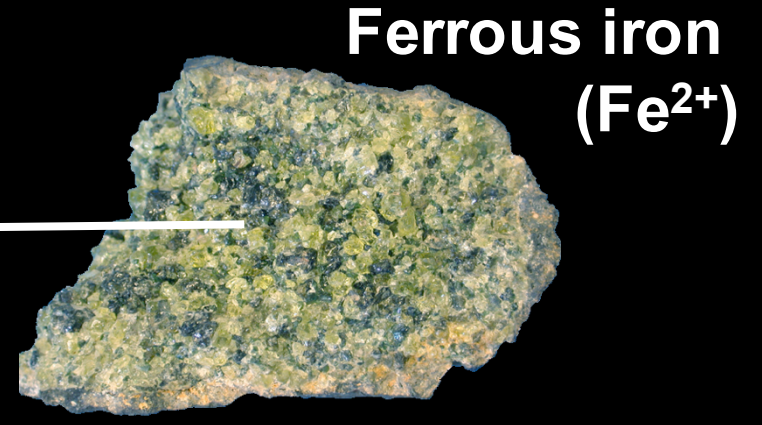
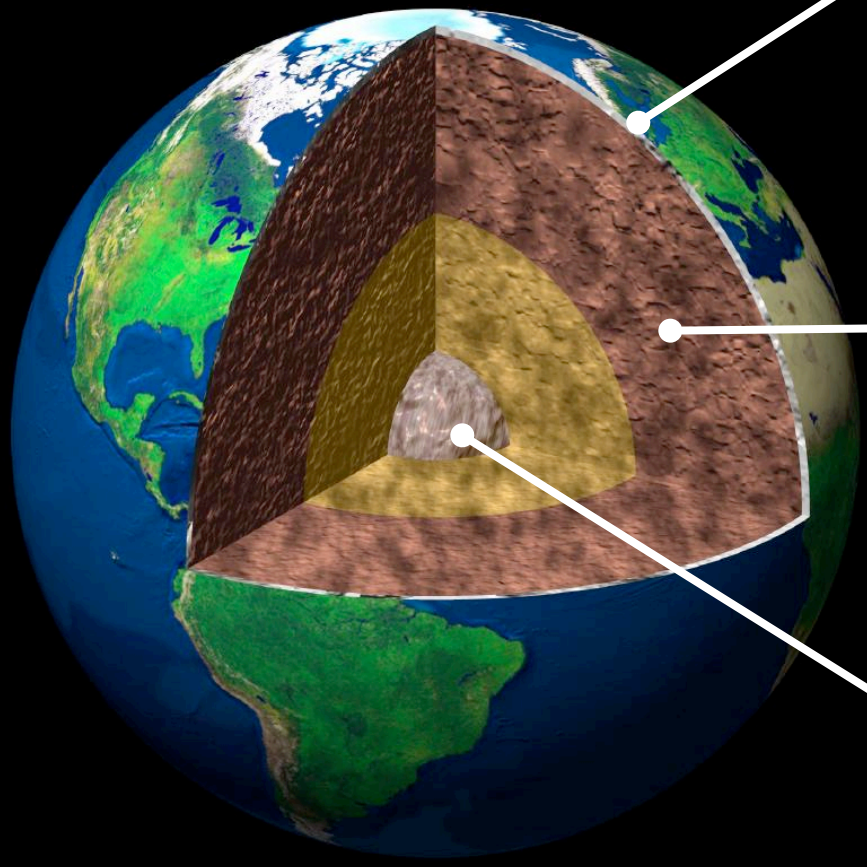
Nicolas Dauphas
dauphas@uchicago.edu



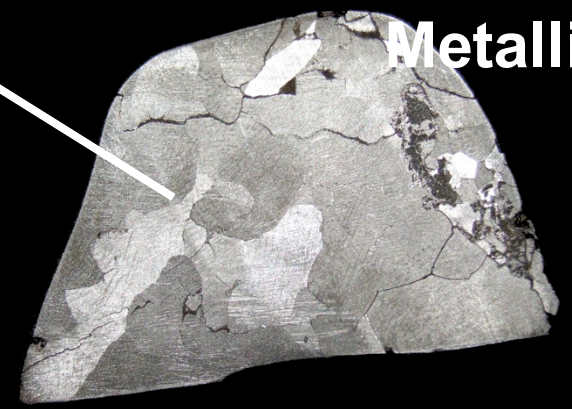
Origins Laboratory
Department of the Geophysical Sciences and Enrico Fermi Institute
The University of Chicago



**Ferric iron
(Fe³⁺)**



**Ferrous iron
(Fe²⁺)**



**Metallic iron
(Fe⁰)**

Dauphas et al. (2017)

Primer on isotopic fractionation

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

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

Example:
15.6994 vs. 15.6979
=0.1‰ fractionation

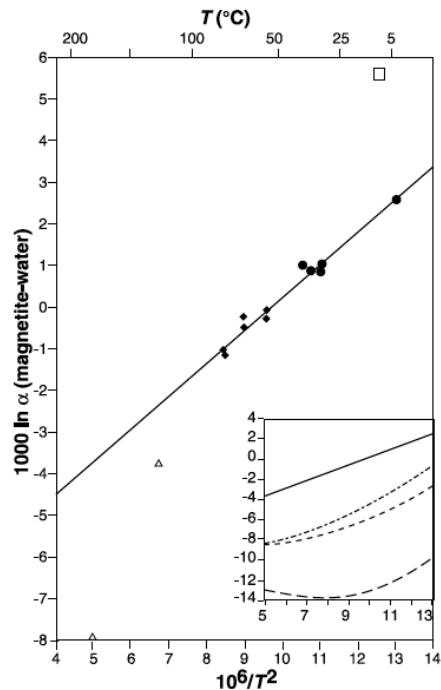
Dauphas & Rouxel (2006) Mass spectrometry and natural variations of iron isotopes.
Mass Spectrom. Rev. 25, 515-550.

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. Bullen⁴

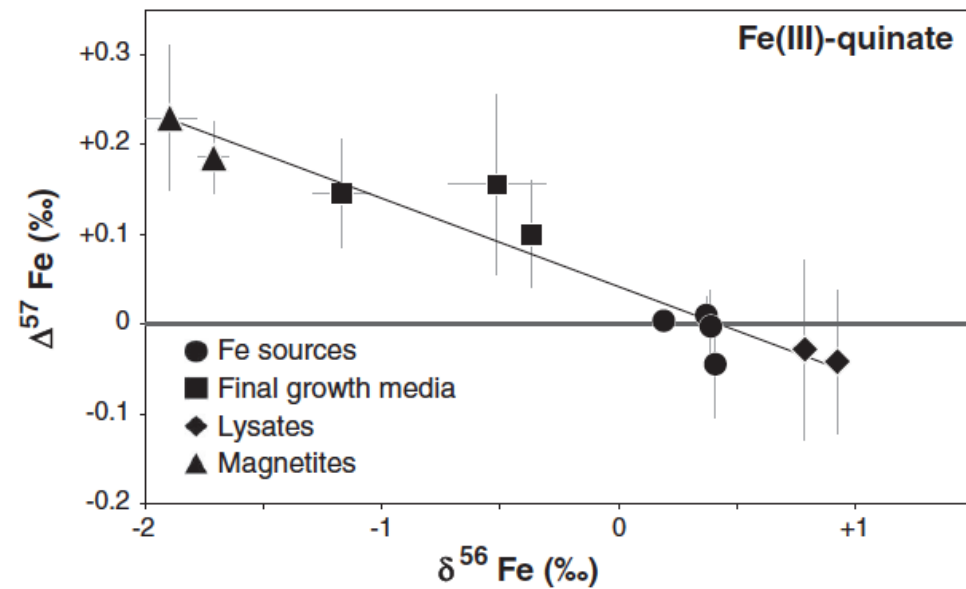
Science 1999



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

Mathieu Amor,^{1,2*} Vincent Busigny,^{1*} Pascale Louvat,¹ Alexandre Gélabert,¹
Pierre Cartigny,¹ Mickaël Durand-Dubief,³ Georges Ona-Nguema,²
Edouard Alphanbéry,^{2,3} Imène Chebbi,³ François Guyot²

Science 2016

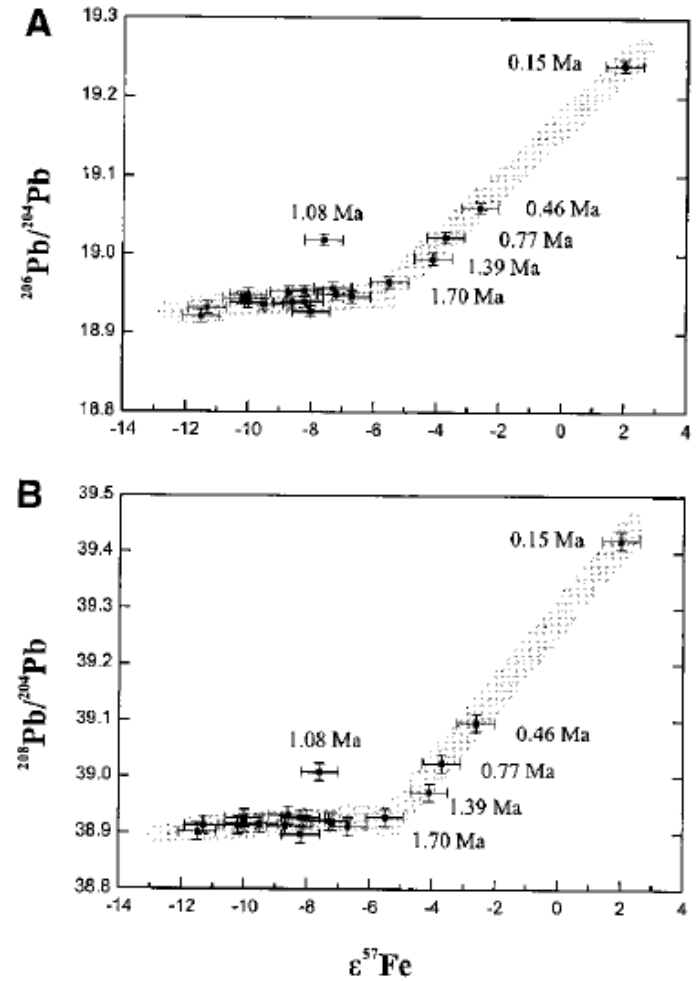


Uses of iron isotopes

Secular Variation of Iron Isotopes in North Atlantic Deep Water

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

Science 2000

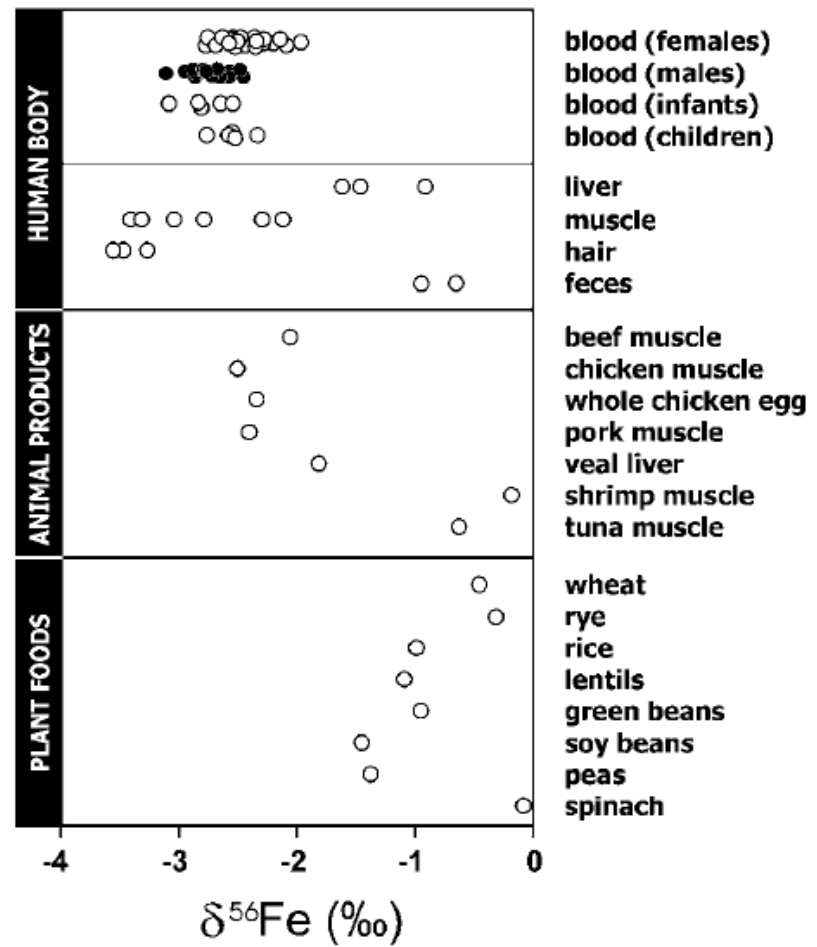


Uses of iron isotopes

Natural Iron Isotope Variations in Human Blood

Thomas Walczyk^{1*} and Friedhelm von Blanckenburg^{2†}

Science 2002

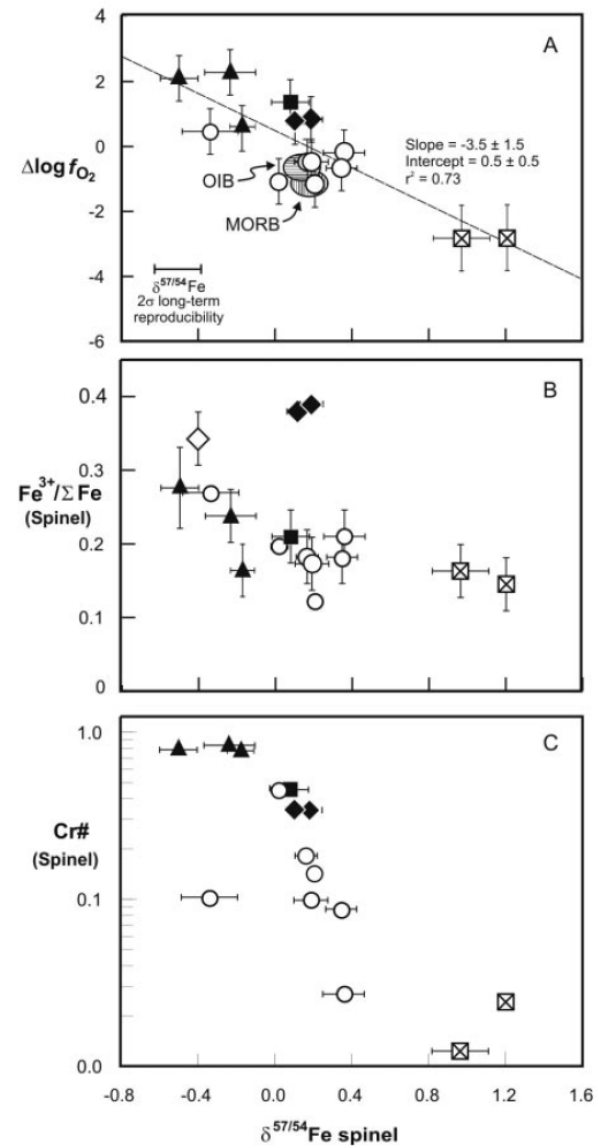


Uses of iron isotopes

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 Burg¹

Science 2004

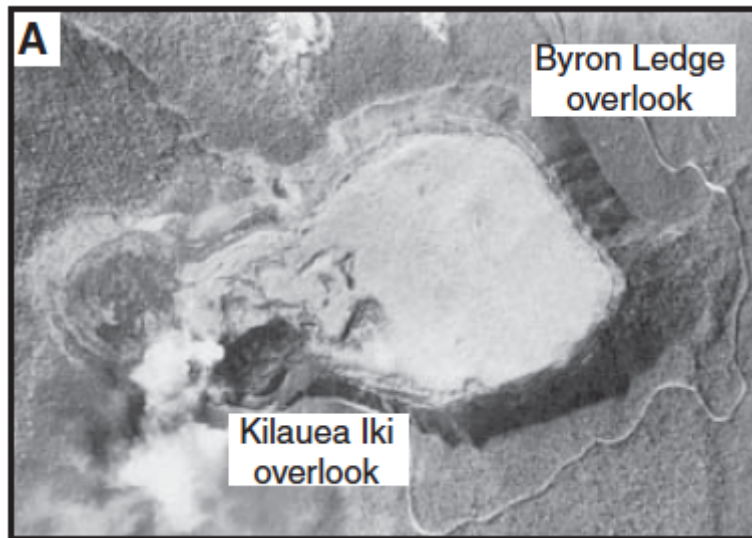
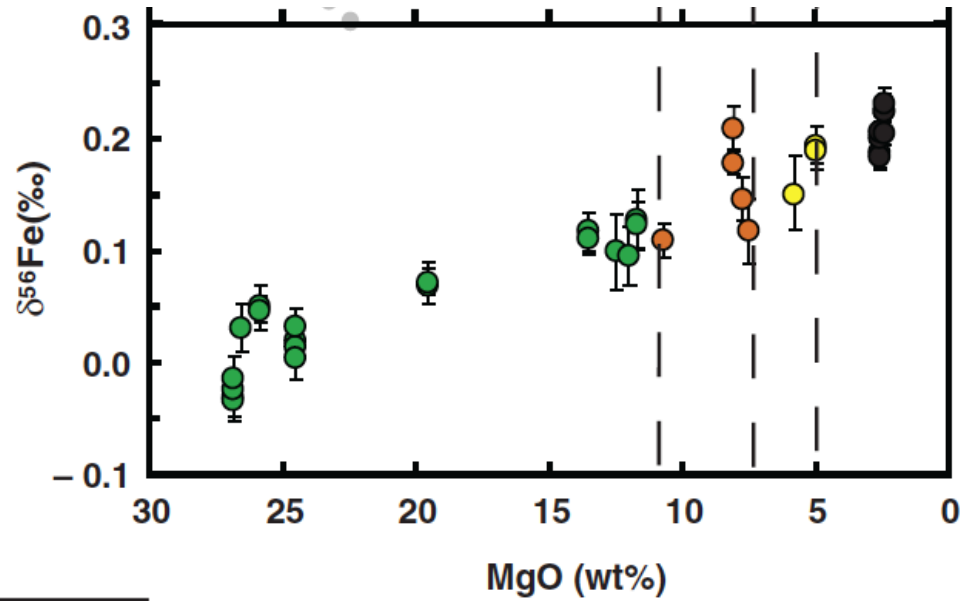


Uses of iron isotopes

Iron Isotope Fractionation During Magmatic Differentiation in Kilauea Iki Lava Lake

Fang-Zhen Teng,^{1*}† Nicolas Dauphas,¹ Rosalind T. Helz²

Science 2008

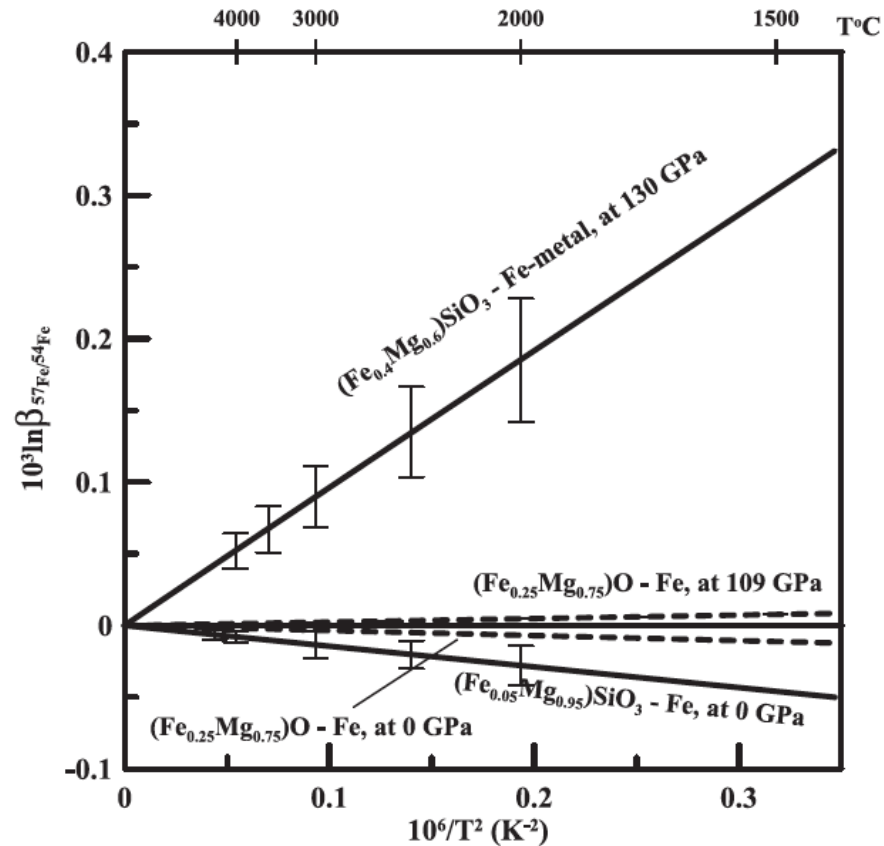


Uses of iron isotopes

Equilibrium Iron Isotope Fractionation at Core-Mantle Boundary Conditions

Veniamin B. Polyakov

Science 2009

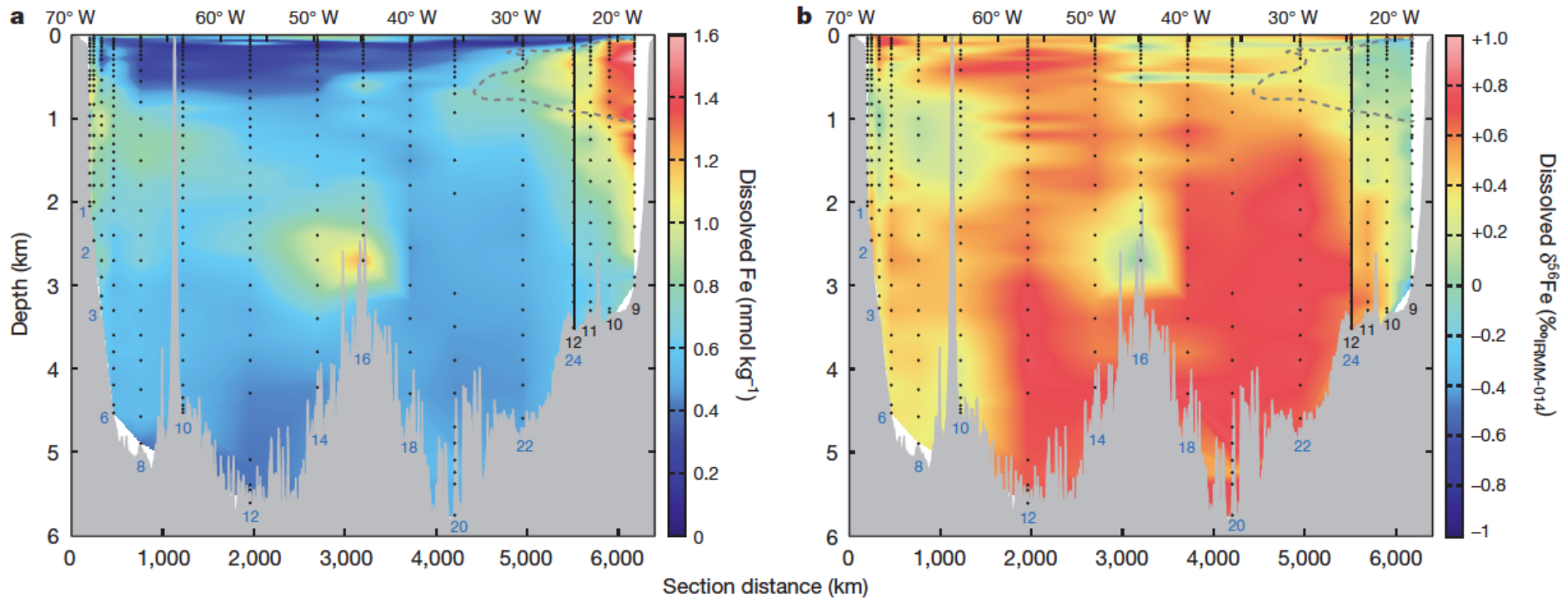


Uses of iron isotopes

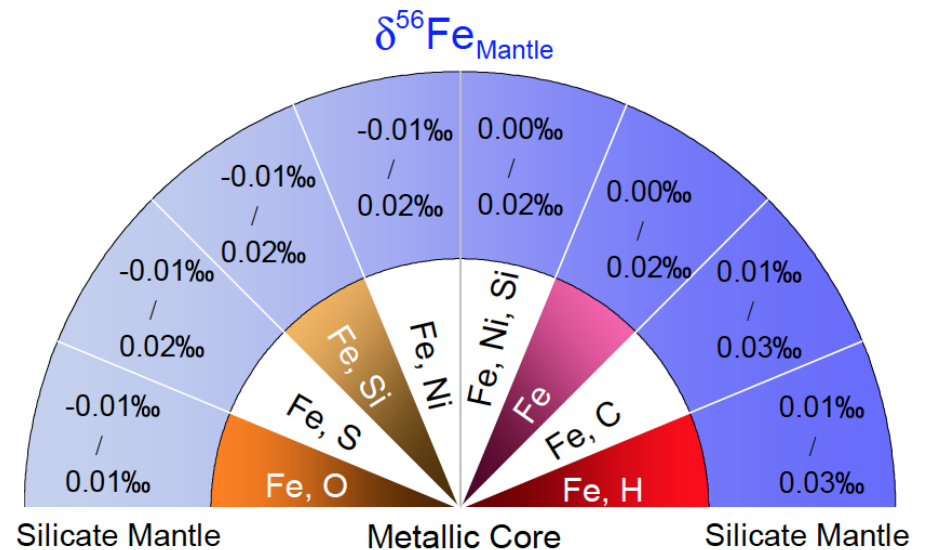
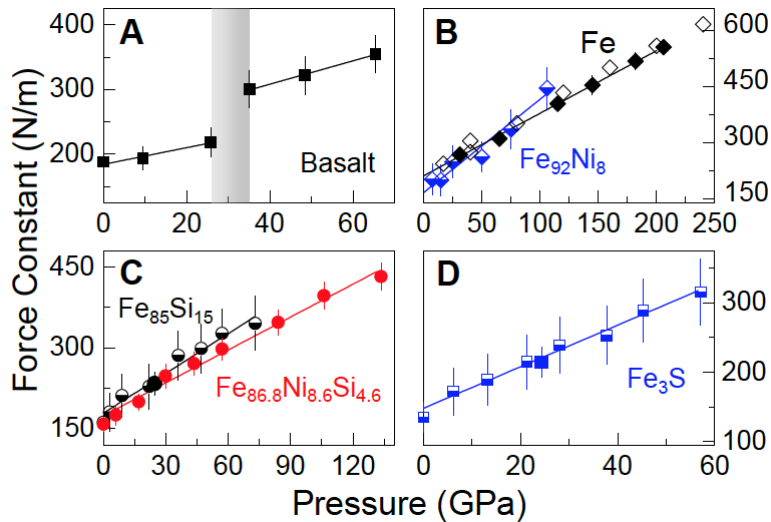
Quantification of dissolved iron sources to the North Atlantic Ocean

Tim M. Conway^{1†} & Seth G. John¹

Nature 2014



Uses of iron isotopes



Science 2016

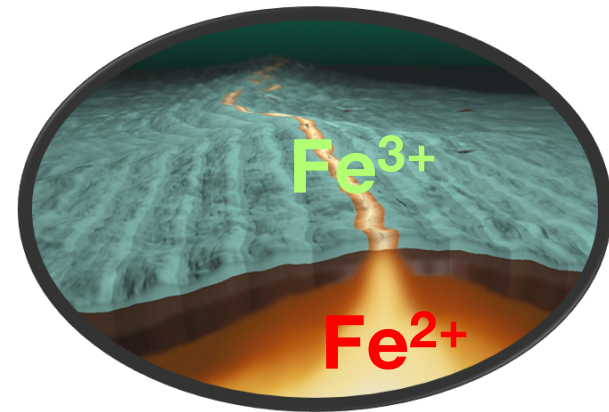
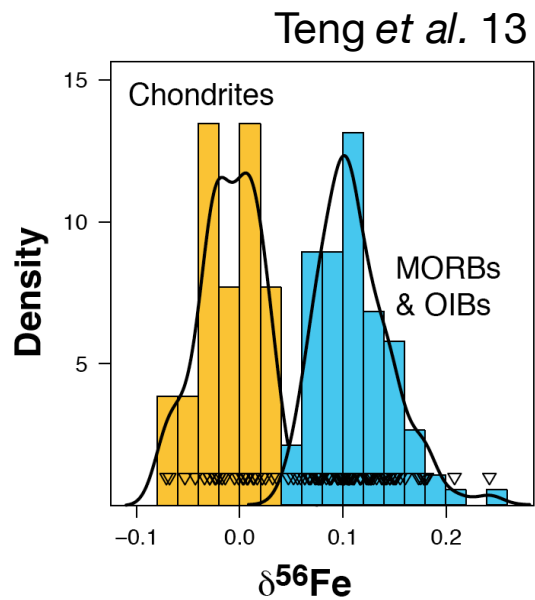
Pressure-dependent isotopic composition of iron alloys

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. Mao⁵

Nature Communications 2016

Liu et al. (in revision)

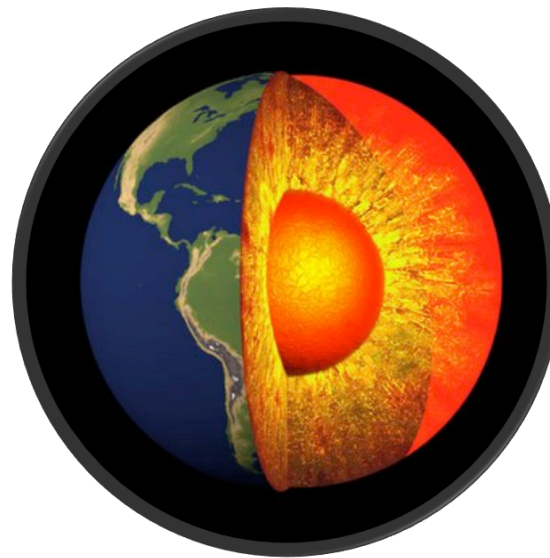
Motivation



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

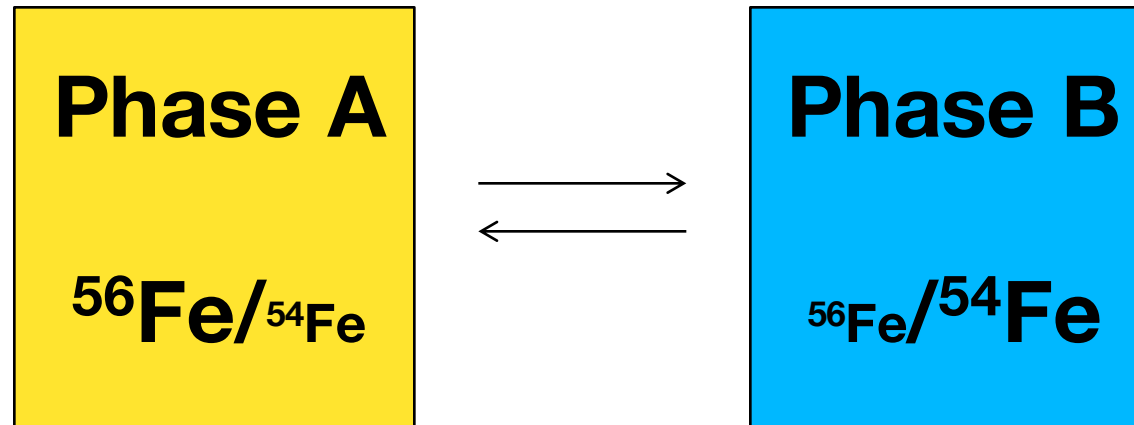


Evaporation
(Poitrasson *et al.* 04)



Metal-silicate partitioning
(Polyakov 09)

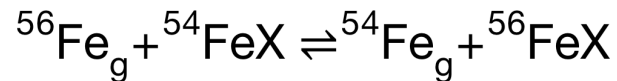
Equilibrium isotopic fractionation



How do iron isotopes partition between coexisting phases at equilibrium?

Equilibrium isotopic fractionation

FeX vs. Fe_g



$$K_{\text{eq}} = \frac{[^{54}\text{Fe}_g][^{56}\text{FeX}]}{[^{56}\text{Fe}_g][^{54}\text{FeX}]} = \frac{[^{56}\text{FeX}]/[^{54}\text{FeX}]}{[^{56}\text{Fe}_g]/[^{54}\text{Fe}_g]} = \frac{(^{56}\text{Fe}/^{54}\text{Fe})_{\text{FeX}}}{(^{56}\text{Fe}/^{54}\text{Fe})_{\text{Fe}_g}}$$

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

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

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

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

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

Urey (1947); Bigeleisen and Mayer (1947)

Equilibrium isotopic fractionation

$$Q_{\text{vib},i} = \frac{e^{-\frac{hv_i}{2kT}}}{1 - e^{-\frac{hv_i}{kT}}}$$

$$K_{\text{eq}} = \prod_i \frac{u'_i}{u_i} \frac{e^{-u'_i/2}}{1 - e^{-u'_i}} \frac{1 - e^{-u_i}}{e^{-u_i/2}}$$
$$u_i = \frac{hv_i}{kT}$$

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

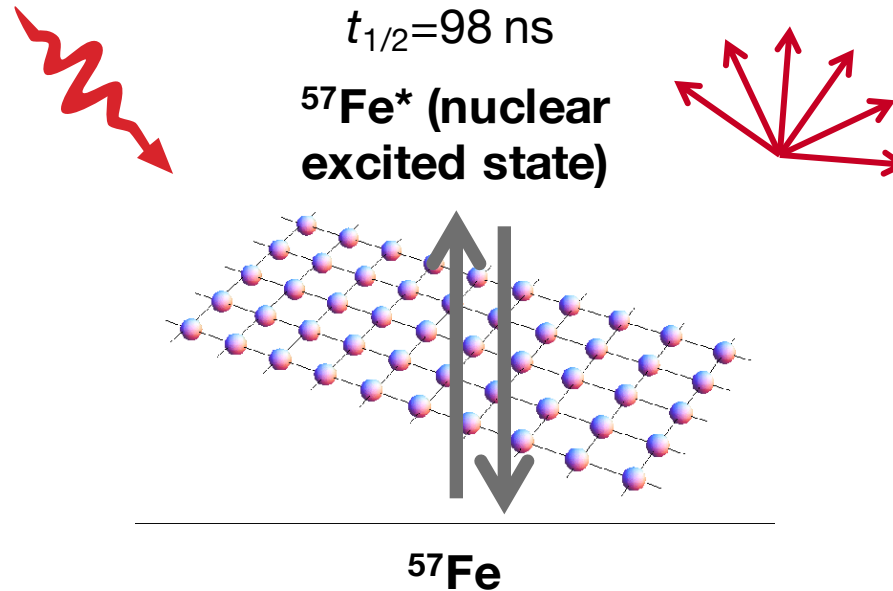
Reduced partition function ratio = β

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



β -factors in solids (for harmonic potential)

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

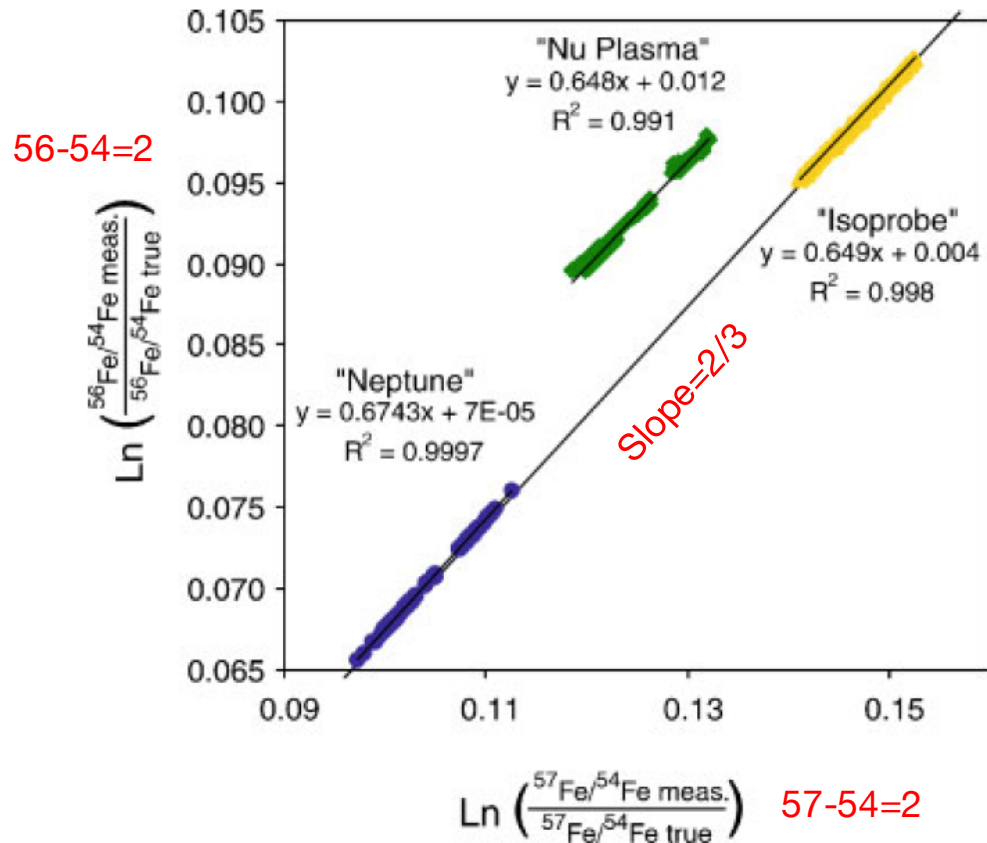
Iron partial phonon density
of states (PDOS)

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

Temperature at which
one wants to calculate β

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

Mass-dependent fractionation



Dauphas and Rouxel (2006)

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:

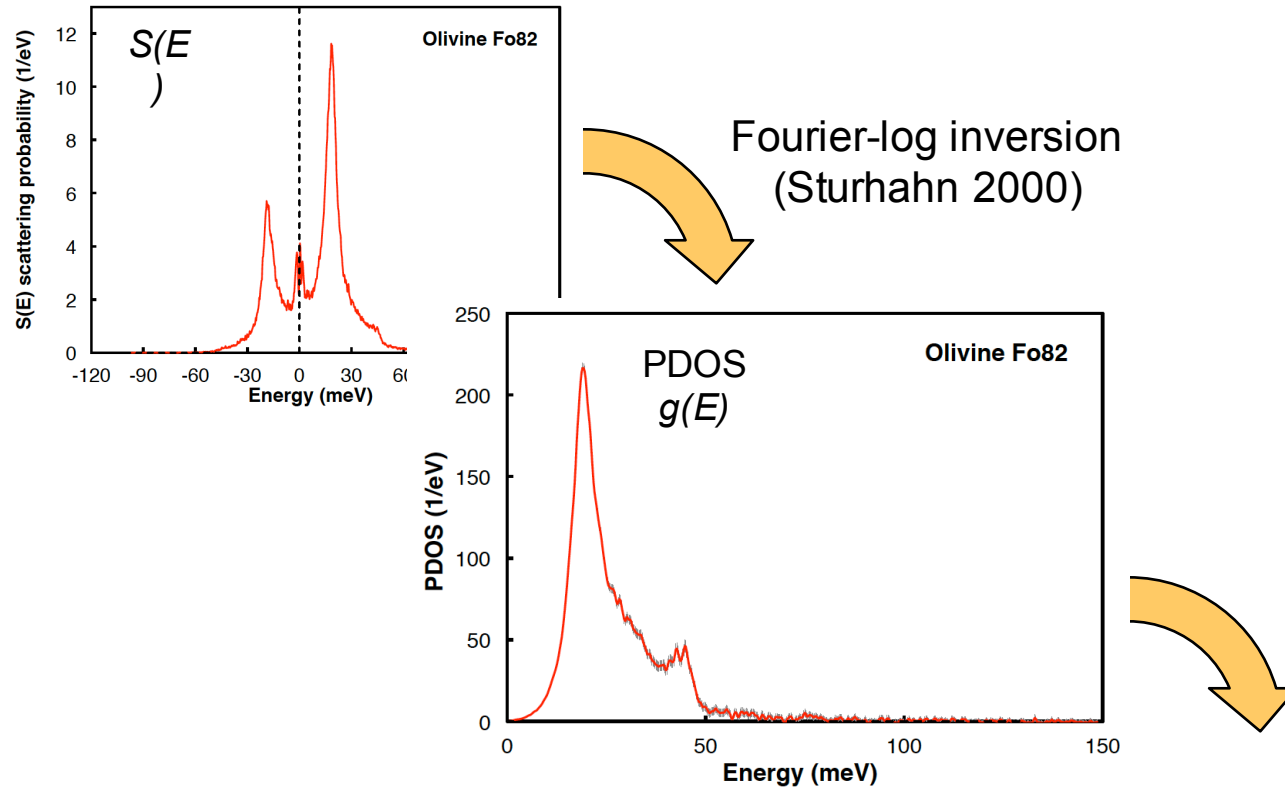
$$1000 \ln \beta_{I/I^*} \simeq 1000 \left(\frac{M}{M^*} - 1 \right) \left(\frac{m_2^g}{8k^2T^2} - \frac{m_4^g}{480k^4T^4} + \frac{m_6^g}{20,160k^6T^6} \right)$$

with

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

j^{th} moment of g

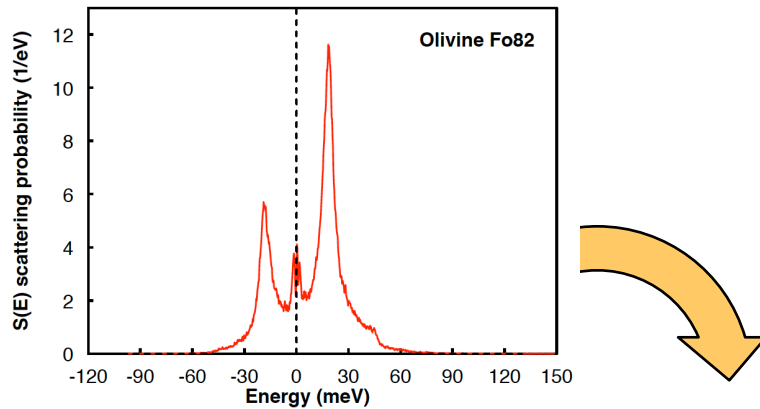
β -factors in solids



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

β -factors in solids

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



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

$$\times \frac{1}{E_r} \left[\frac{R_3^S}{8k^2 T^2} - \frac{R_5^S - 10R_2^S R_3^S}{480k^4 T^4} + \frac{R_7^S + 210(R_2^S)^2 R_3^S - 35R_3^S R_4^S - 21R_2^S R_5^S}{20,160k^6 T^6} \right]$$

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

High temperature approximation

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

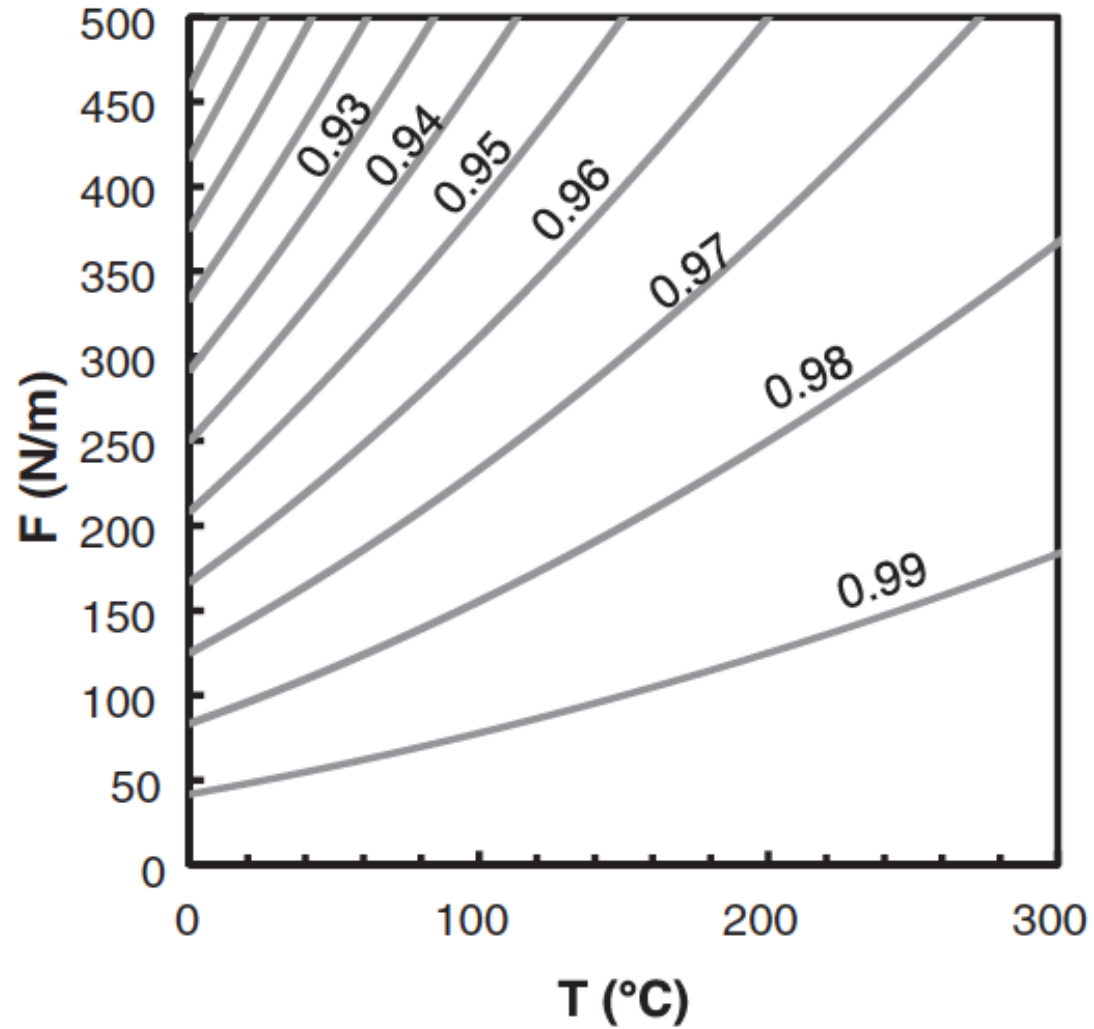
$$1000 \times \ln \beta_{I/I^*} = 1000 \left(\frac{1}{M^*} - \frac{1}{M} \right) \frac{\hbar^2}{8k^2 T^2} \langle F \rangle$$

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

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

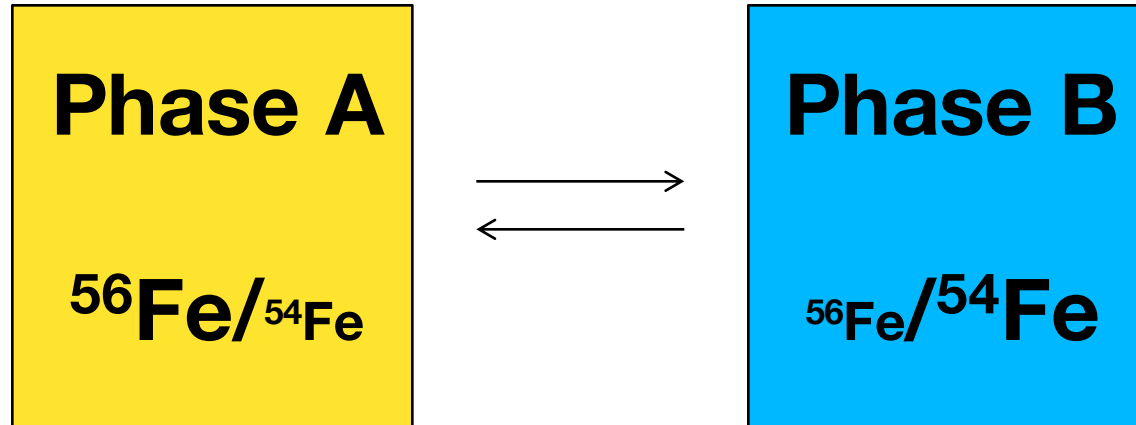


High temperature approximation



A good approximation for iron

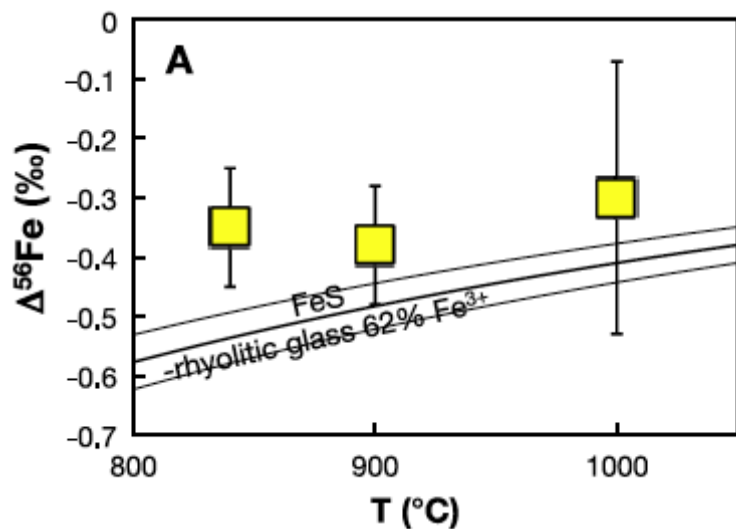
Equilibration experiments



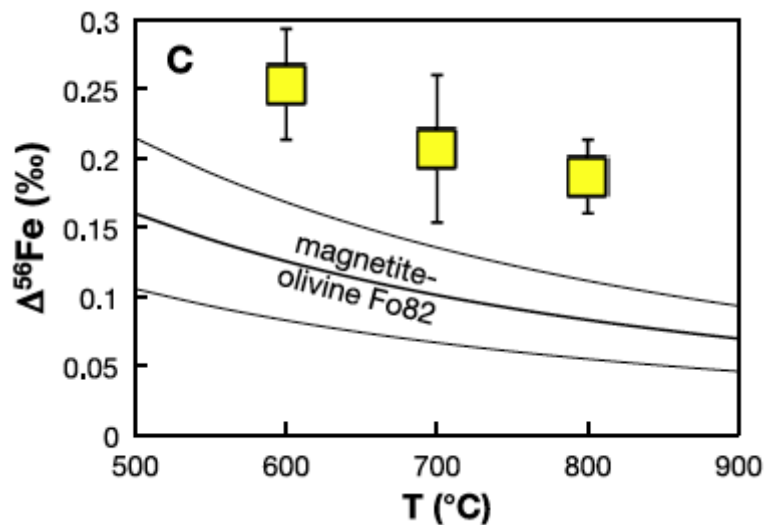
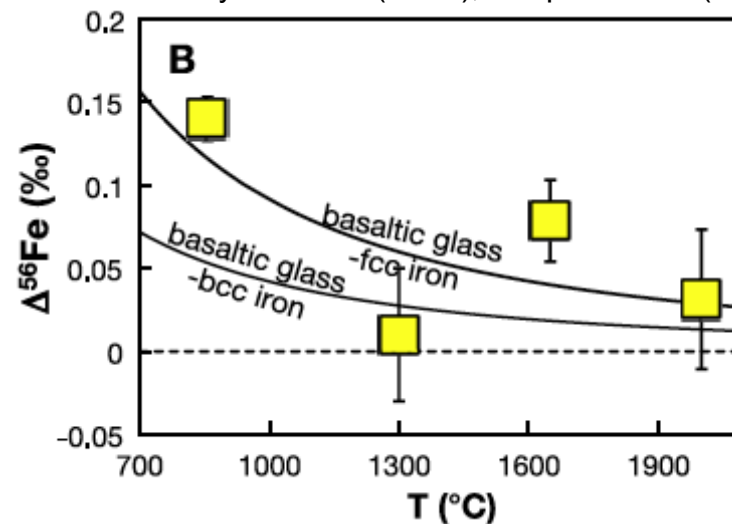
Method comparison

Data: Schuessler et al. (2007)

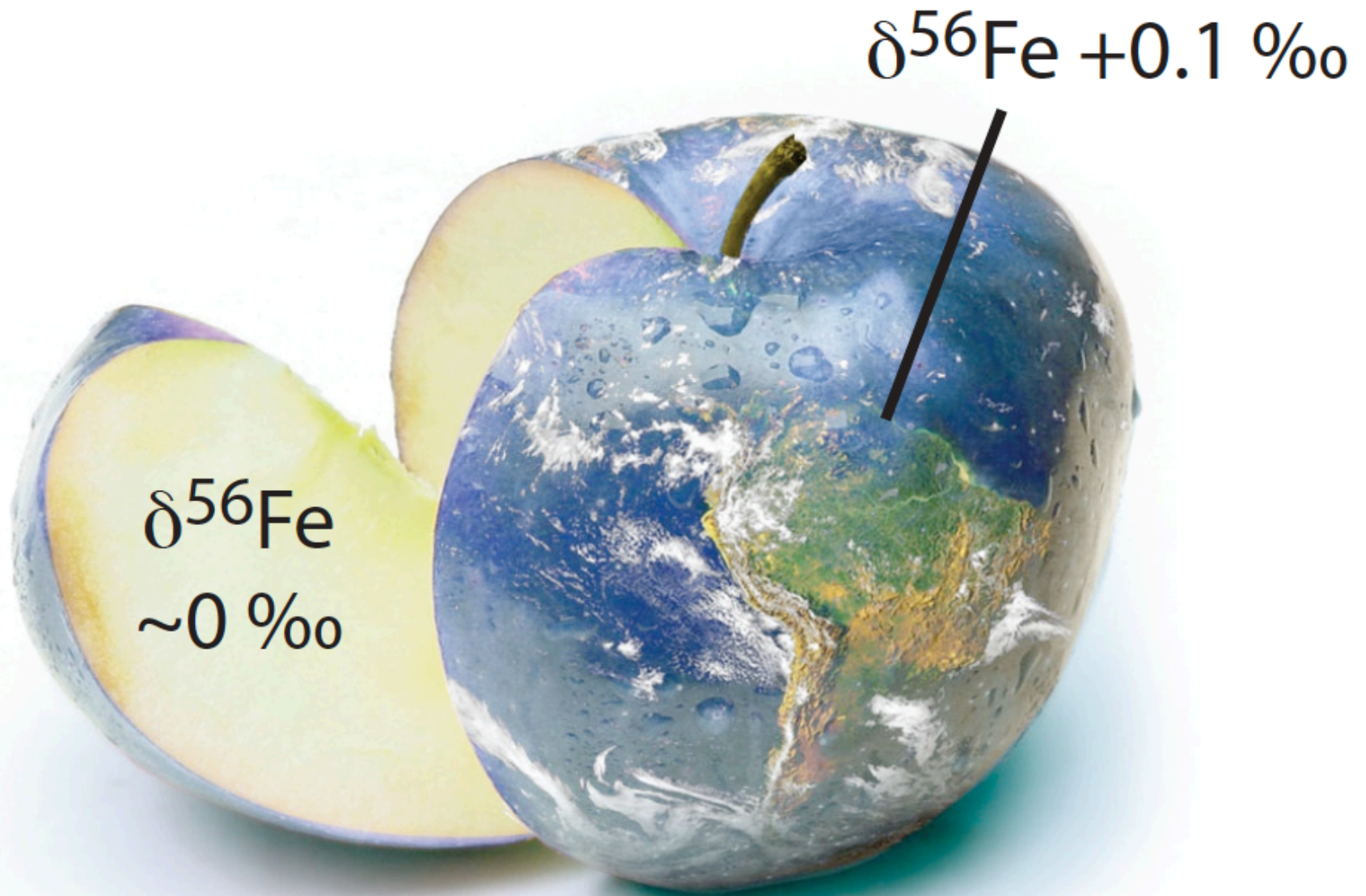
FC: Krawczynski et al. (2014), Dauphas et al. (2014)



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)

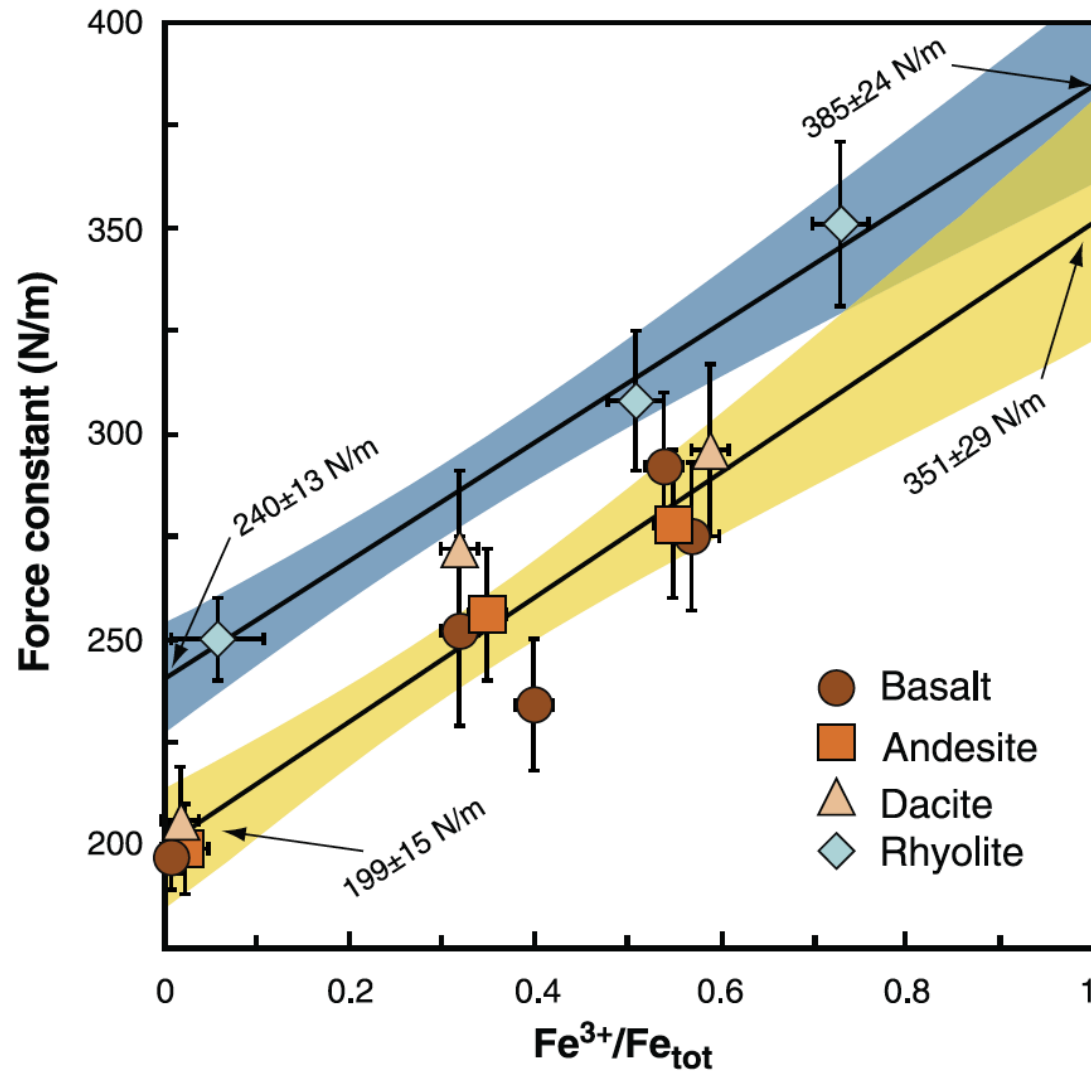


Data: Shahar et al. (2008)
FC: Polyakov et al. (2007), Dauphas et al. (2012, 2014)



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

Force constant results

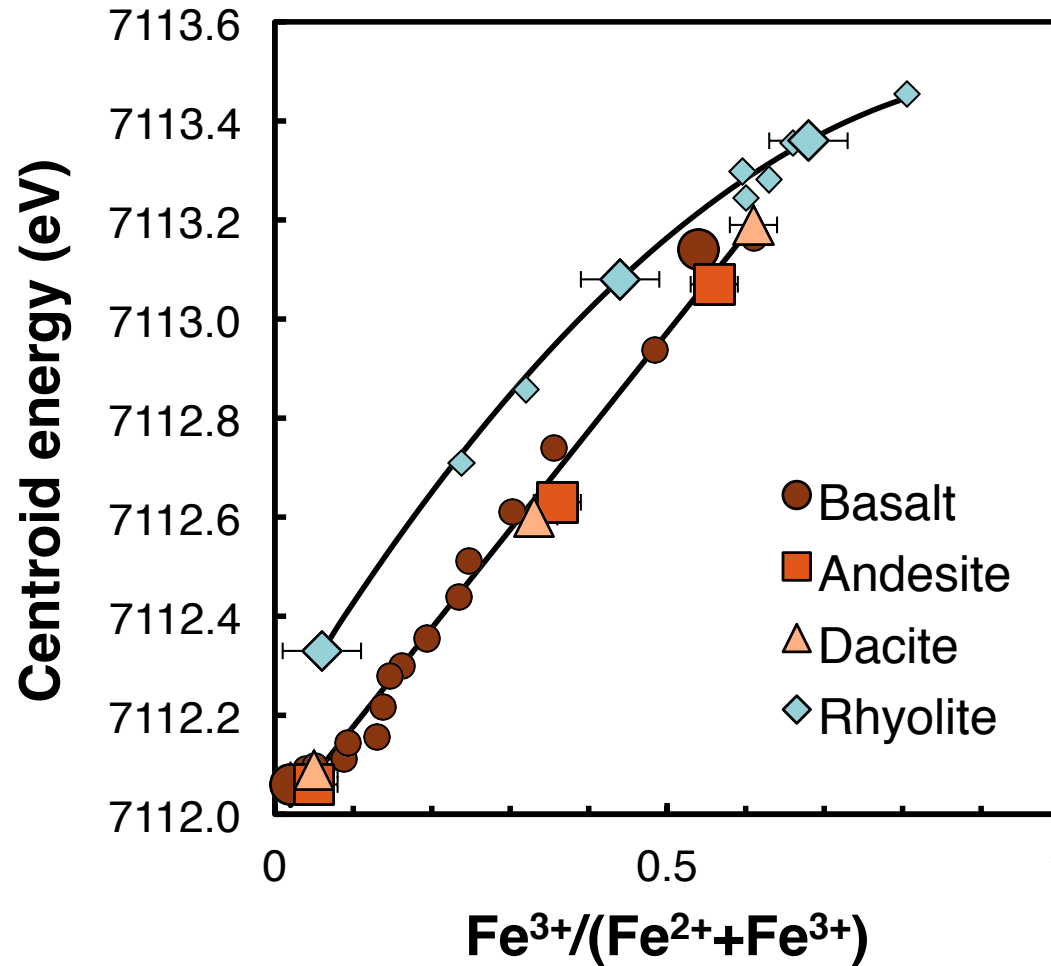


Dauphas et al. (2014)



Redox and structural controls in glasses

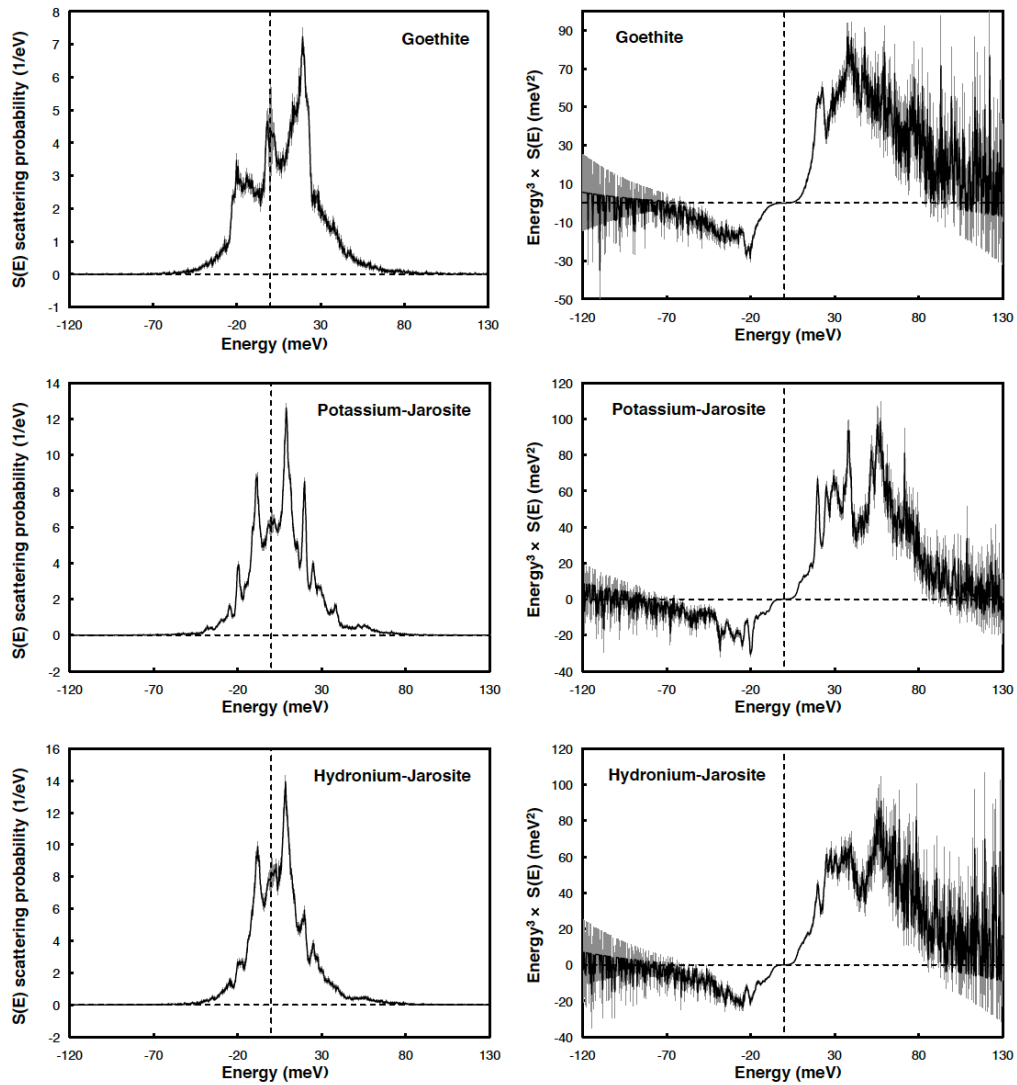
XANES



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

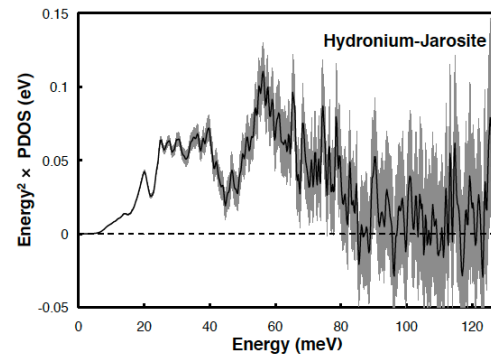
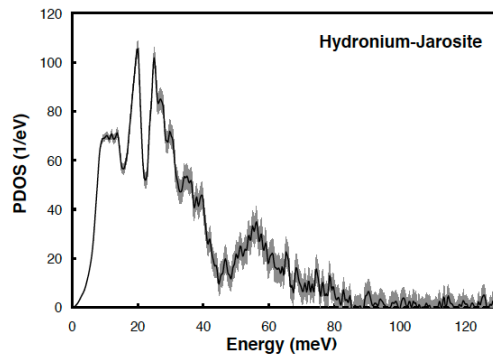
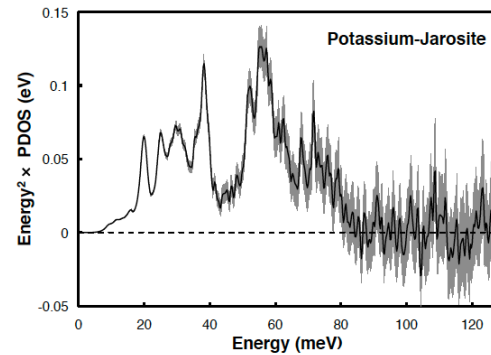
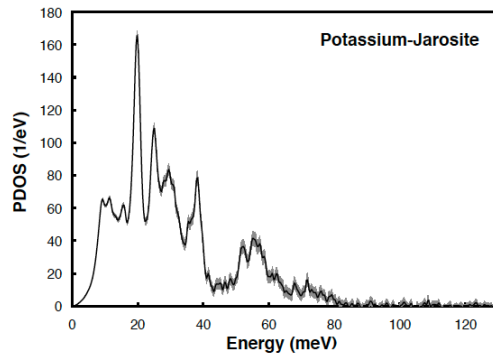
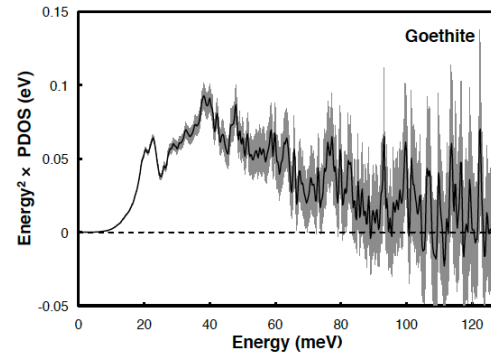
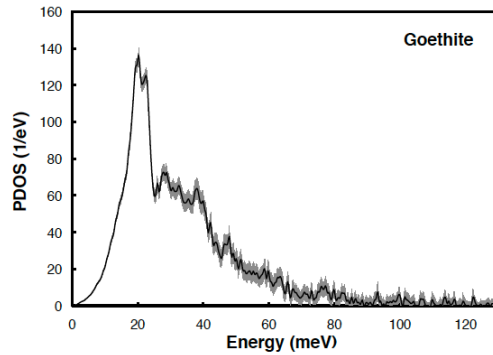
Difficulties with force constant measurements

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



Difficulties with force constant measurements

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

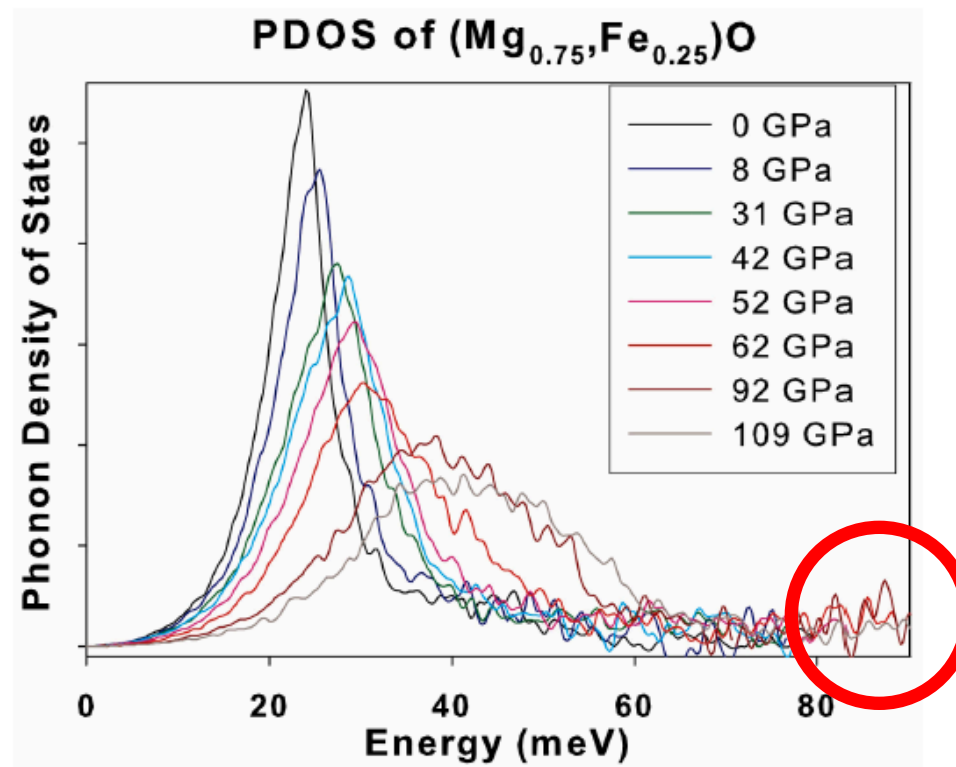


A word of caution with published data

Equilibrium Iron Isotope Fractionation at Core-Mantle Boundary Conditions

Veniamin B. Polyakov

13 FEBRUARY 2009 VOL 323 SCIENCE www.sciencemag.org



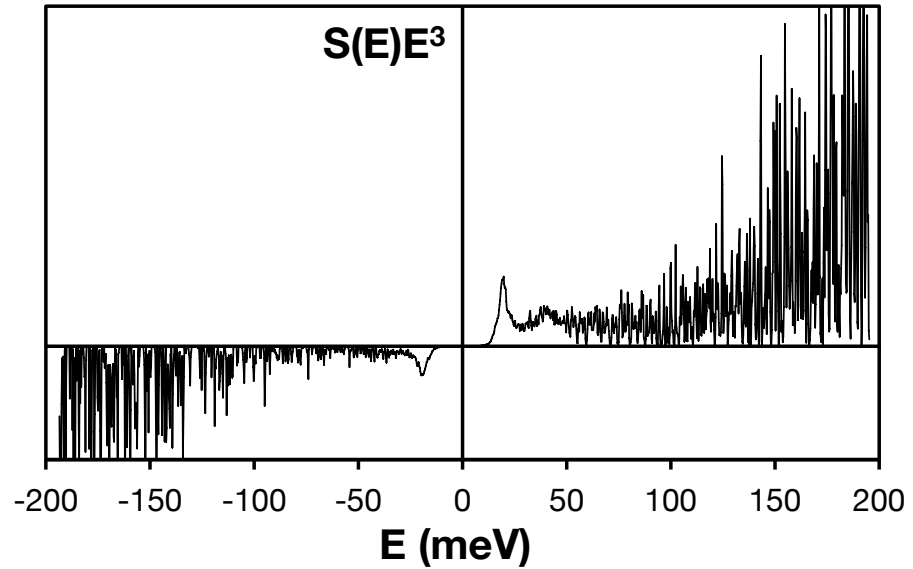
Lin et al. (2006)



Unaccounted baseline in NRIXS

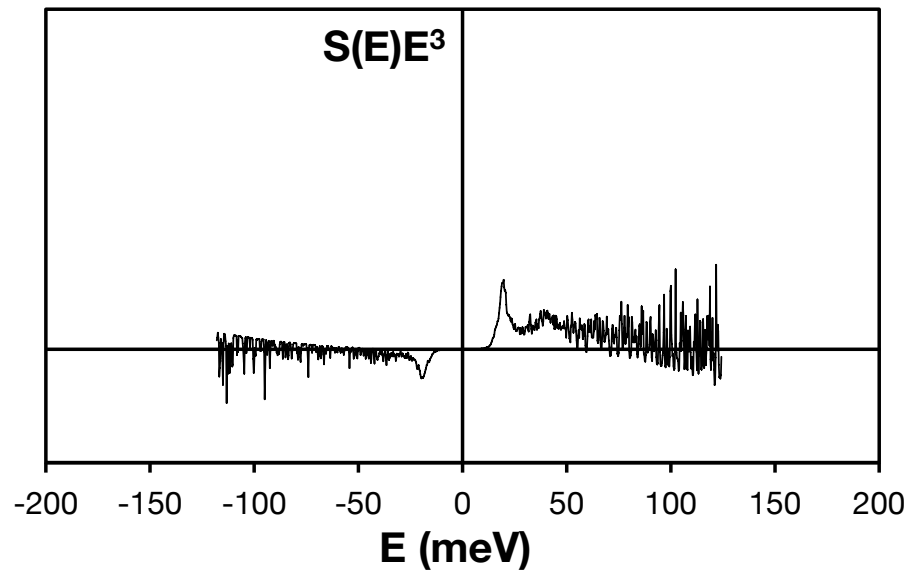
No baseline subtraction

$$\langle F \rangle = 968 \pm 128 \text{ N/m}$$

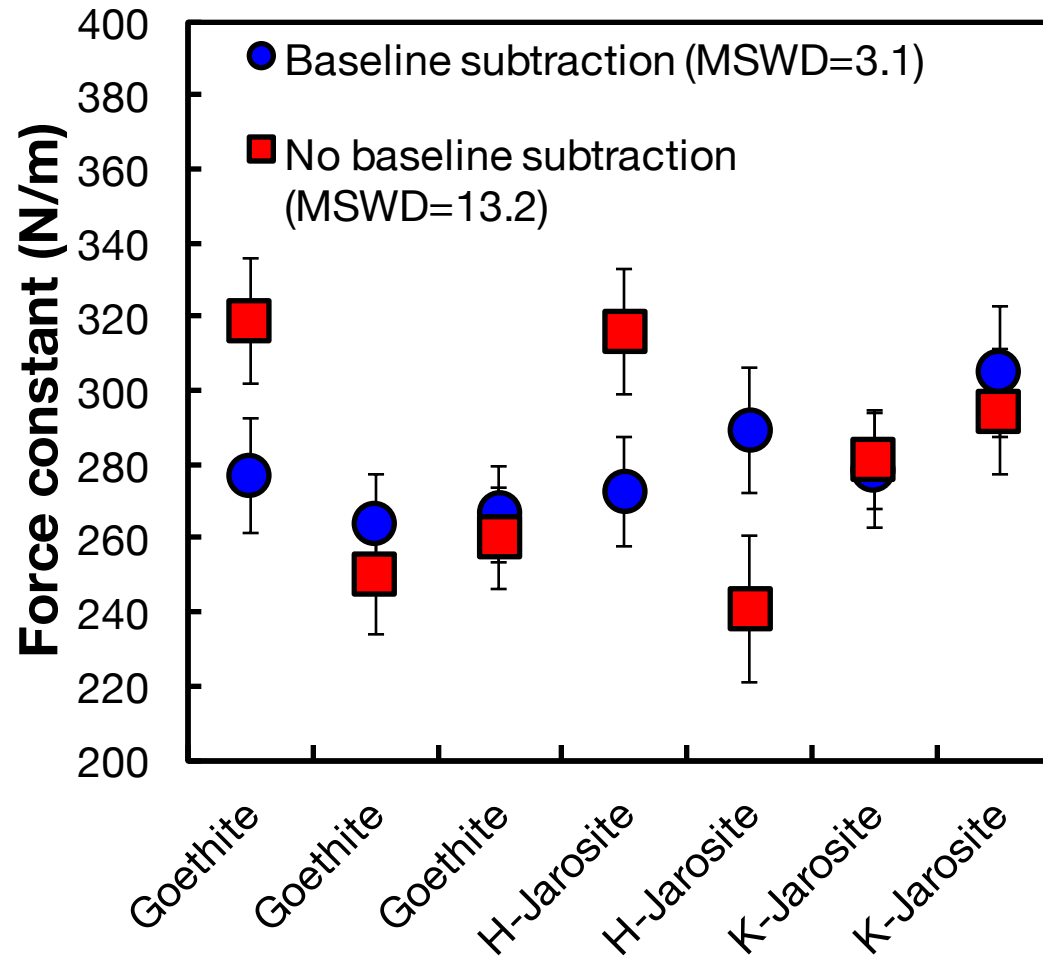


Baseline subtraction
with SciPhon

$$\langle F \rangle = 213 \pm 36 \text{ N/m}$$



Baseline subtraction



Improves the session-to-session long term reproducibility



Error propagation in derived quantities

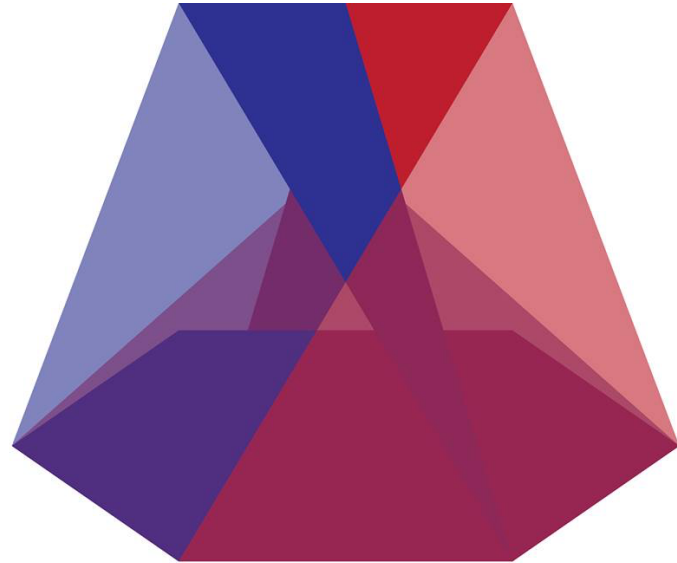
- Counting statistics
- Parameters of the baseline $(a \pm \sigma_a)x + (b \pm \sigma_b)$
- Zero energy bin
- Energy scaling
- Bin-to-bin energy variations

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



Motivations for SciPhon

1. Have a GUI interface
1. Streamline the baseline subtraction procedure
1. Propagate sources of uncertainties other than counting statistics
2. Output quantities directly usable in isotope geochemistry



SciPhon



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

SciPhon 1.0

Select isotope: **Fe-57**

1. Load data

2. Load resolution

3. Deconvolve resolution from data

4. Okay-proceed

5. Elastic peak removal

6. Energy truncation/baseline definition

7. Temperature calculation

8. Calculate DOS

9. Calculate sound velocities

10. Calc. Parameters

11. Export

Background subtraction (cts): 0

Experiment temperature in K: 300

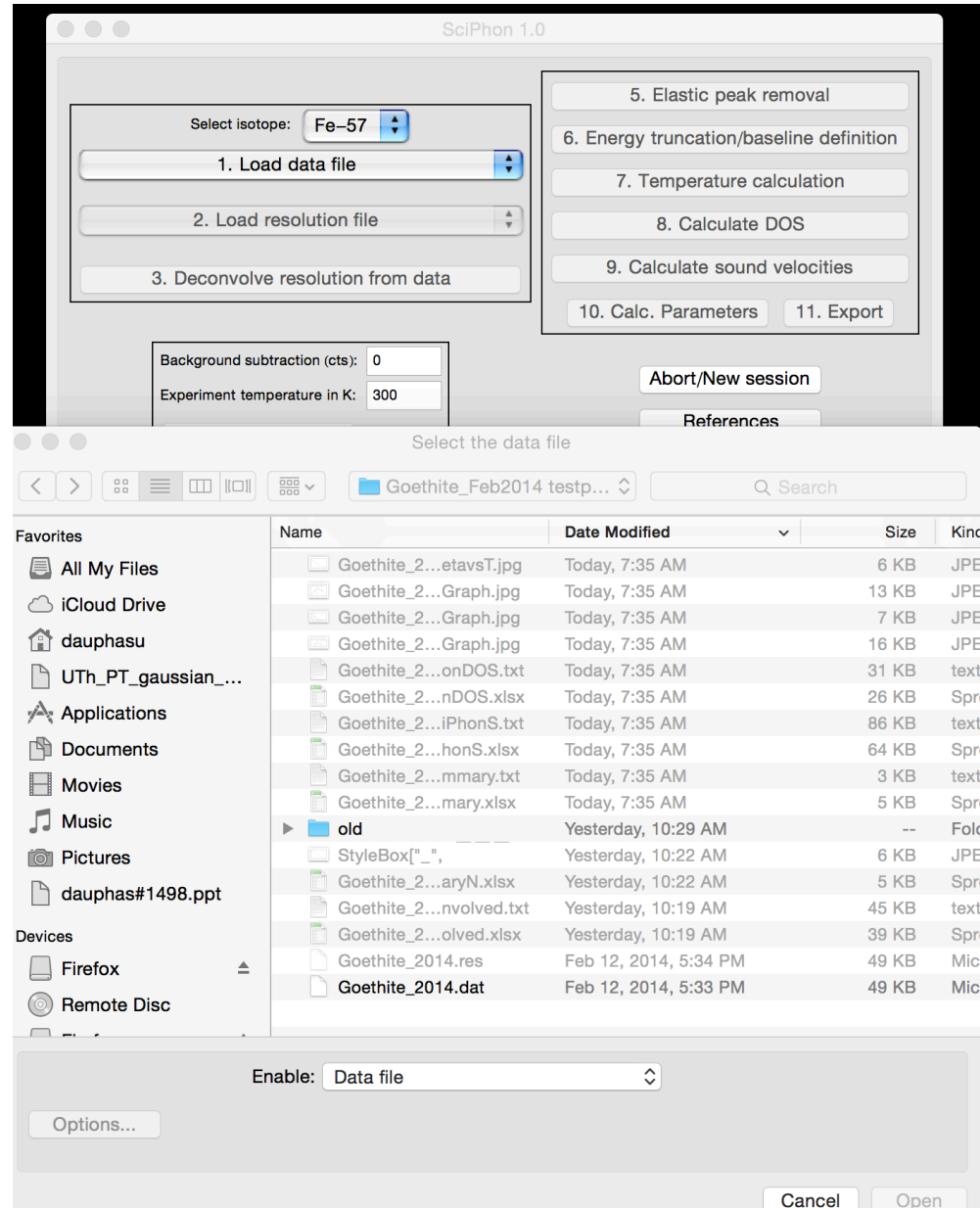
Abort/New session

References

Graphics output:

1 2 3 4

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



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

The image shows the SciPhon 1.0 software interface. The main window has a title bar "SciPhon 1.0" and a "Select isotope:" dropdown set to "Fe-57". The interface is divided into several sections:

- 1. Load data file:** A text field containing the path `/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014/testpoubelle_Nov2014/Goethite_2014.dat`.
- 2. Load resolution file:** A dropdown menu.
- 3. Deconvolve resolution from data:** A button.
- 4. Okay-proceed:** A button.
- Background subtraction (cts):** A text field with the value "0".
- Experiment temperature in K:** A text field with the value "300".
- 5. Elastic peak removal**
- 6. Energy truncation/baseline definition**
- 7. Temperature calculation**
- 8. Calculate DOS**
- 9. Calculate sound velocities**
- 10. Calc. Parameters**
- 11. Export**
- Abort/New session** and **References** buttons.
- Graphics output:** A large empty area with a small navigation bar containing buttons "1", "2", "3", and "4".

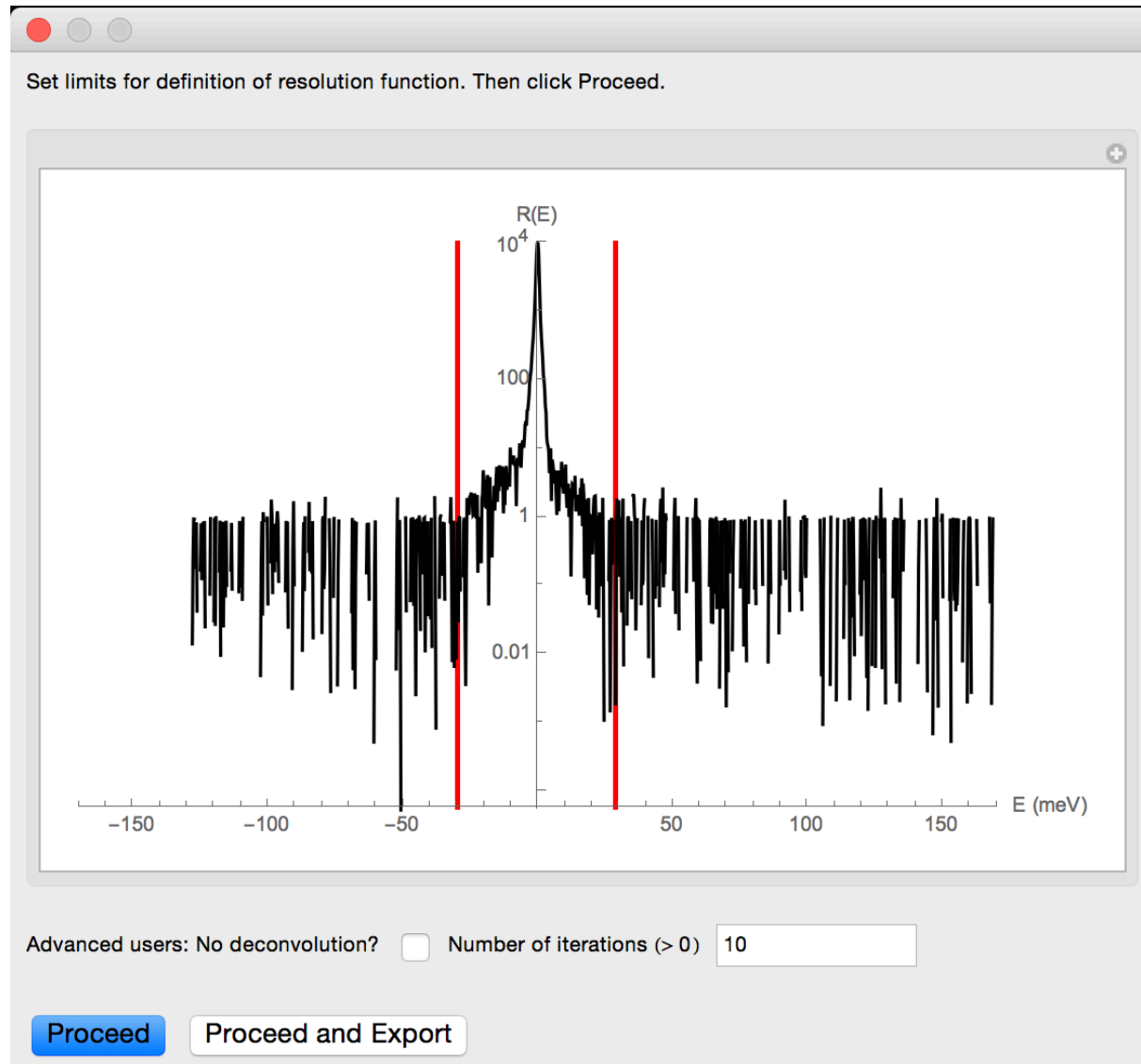
A "Select the resolution file" dialog box is open in the foreground, showing a file browser view of the "Goethite_Feb2014 testp..." directory. The dialog has a search bar and a table of files:

Name	Date Modified	Size	Kind
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	Spre
Goethite_2...iPhonS.txt	Today, 7:35 AM	86 KB	text
Goethite_2...honS.xlsx	Today, 7:35 AM	64 KB	Spre
Goethite_2...mmary.txt	Today, 7:35 AM	3 KB	text
Goethite_2...mary.xlsx	Today, 7:35 AM	5 KB	Spre
old	Yesterday, 10:29 AM	--	Fold
StyleBox["_", ...]	Yesterday, 10:22 AM	6 KB	JPE
Goethite_2...aryN.xlsx	Yesterday, 10:22 AM	5 KB	Spre
Goethite_2...nolved.txt	Yesterday, 10:19 AM	45 KB	text
Goethite_2...olved.xlsx	Yesterday, 10:19 AM	39 KB	Spre
Goethite_2014.res	Feb 12, 2014, 5:34 PM	49 KB	Mic
Goethite_2014.dat	Feb 12, 2014, 5:33 PM	49 KB	Mic

At the bottom of the dialog, there is an "Enable:" section with a dropdown menu set to "Resolution file" and an "Options..." button. The dialog has "Cancel" and "Open" buttons at the bottom right.

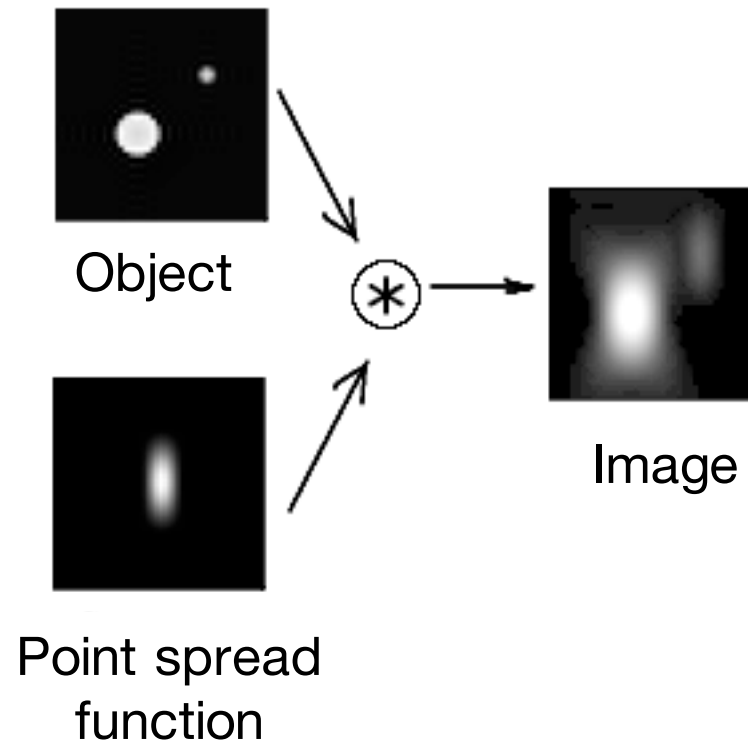


Deconvolution of the resolution from the data using the steepest descent algorithm



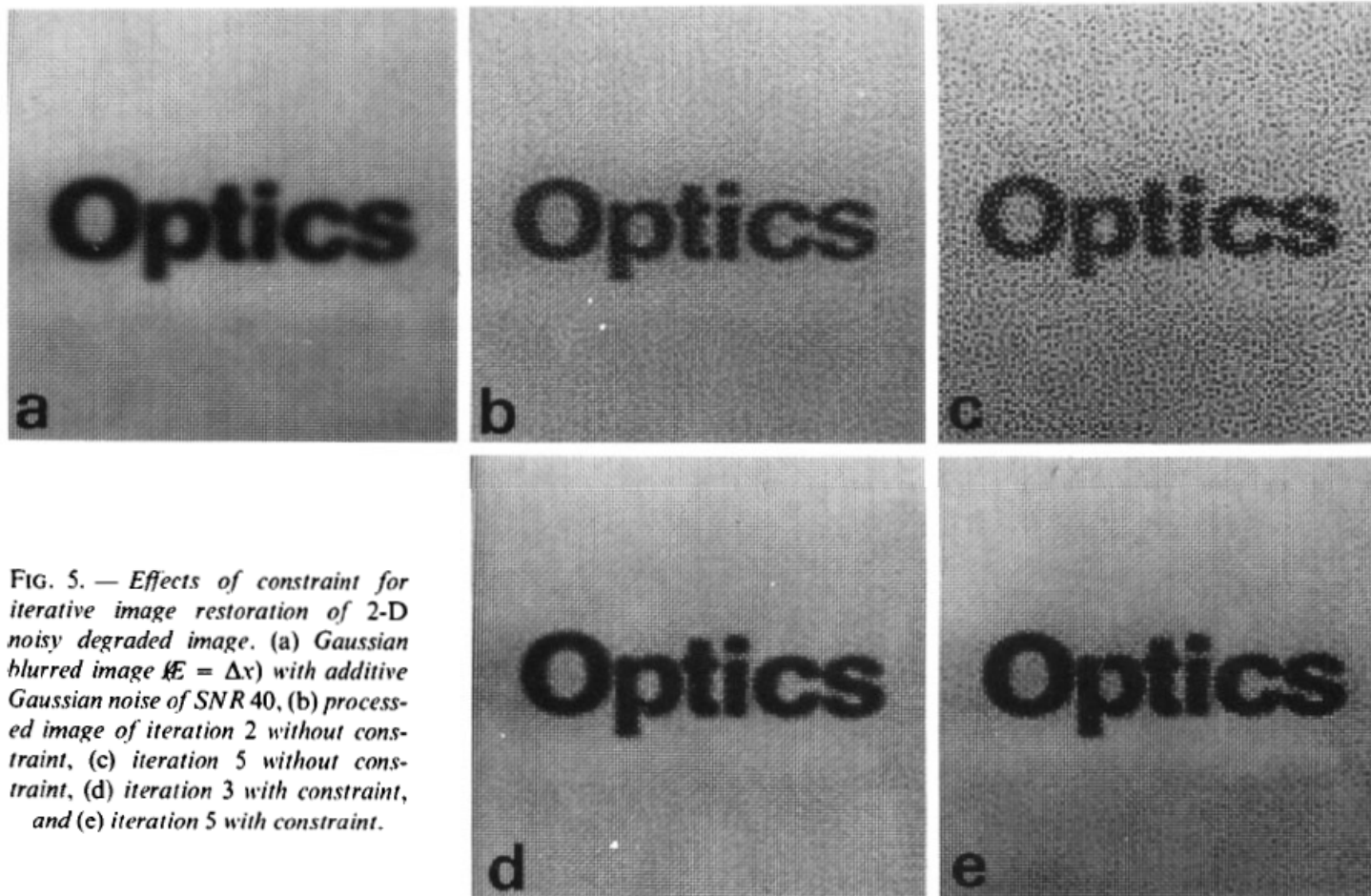


Deconvolution





Deconvolution



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

SciPhon 1.0

Select isotope: Fe-57

1. Load data file
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014
testpoubelle_Nov2014/Goethite_2014.dat

2. Load resolution file
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014
testpoubelle_Nov2014/Goethite_2014.res

3. Deconvolve resolution from data

Background subtraction (cts): 0

Experiment temperature in K: 300

4. Okay-proceed

5. Elastic peak removal

6. Energy truncation/baseline definition

7. Temperature calculation

8. Calculate DOS

9. Calculate sound velocities

10. Calc. Parameters 11. Export

Abort/New session

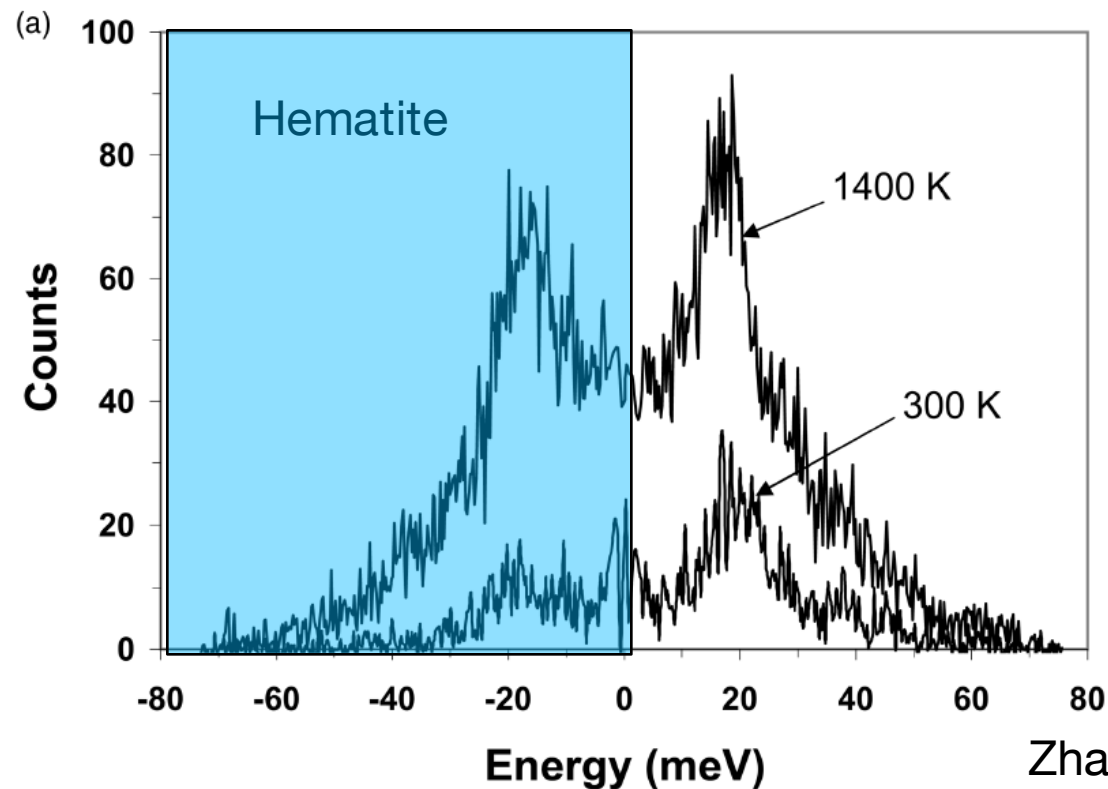
References

Graphics output:

1 2 3 4

Detailed balance

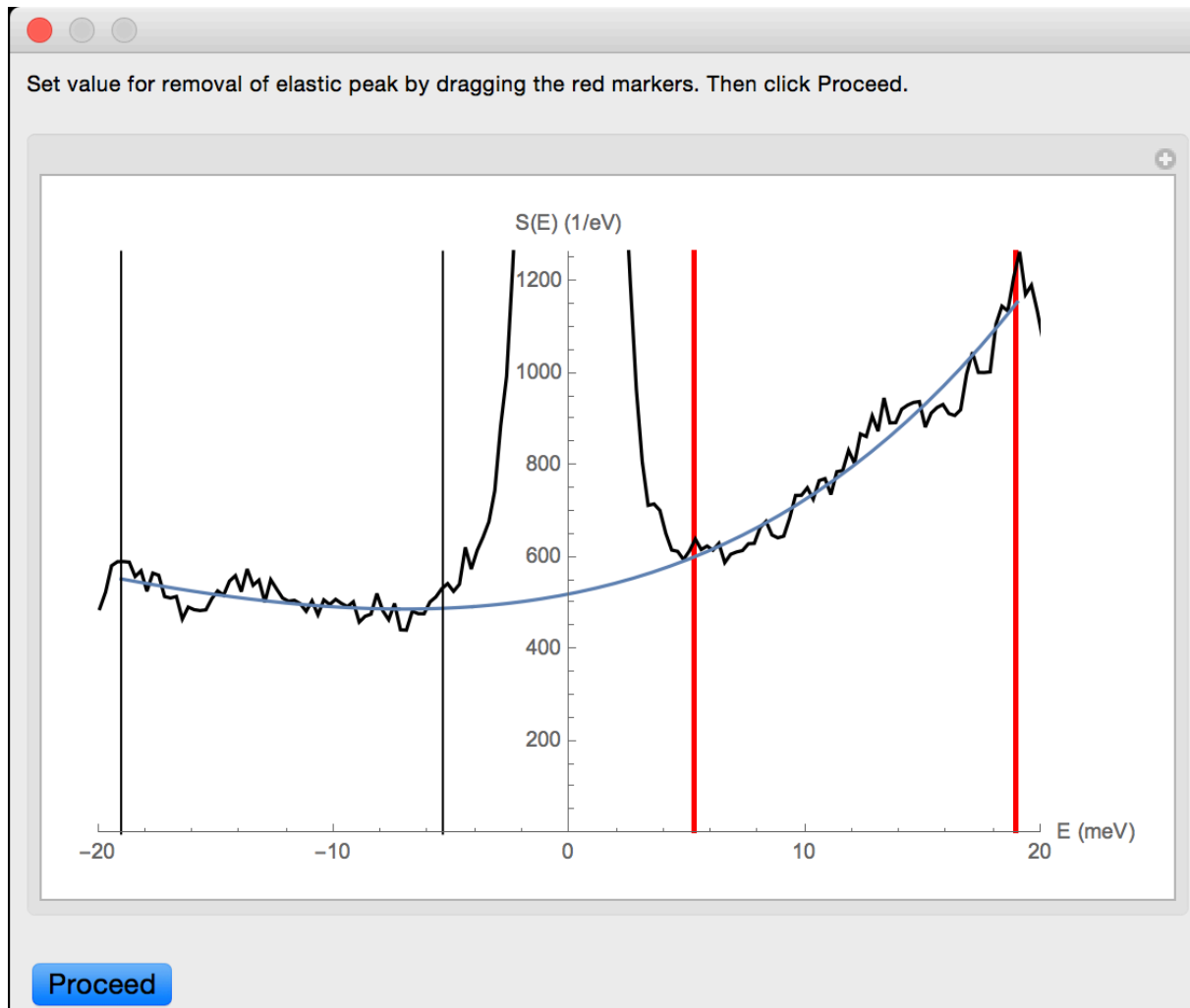
$$\frac{I(E)}{I(-E)} = e^{E/kT}$$



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



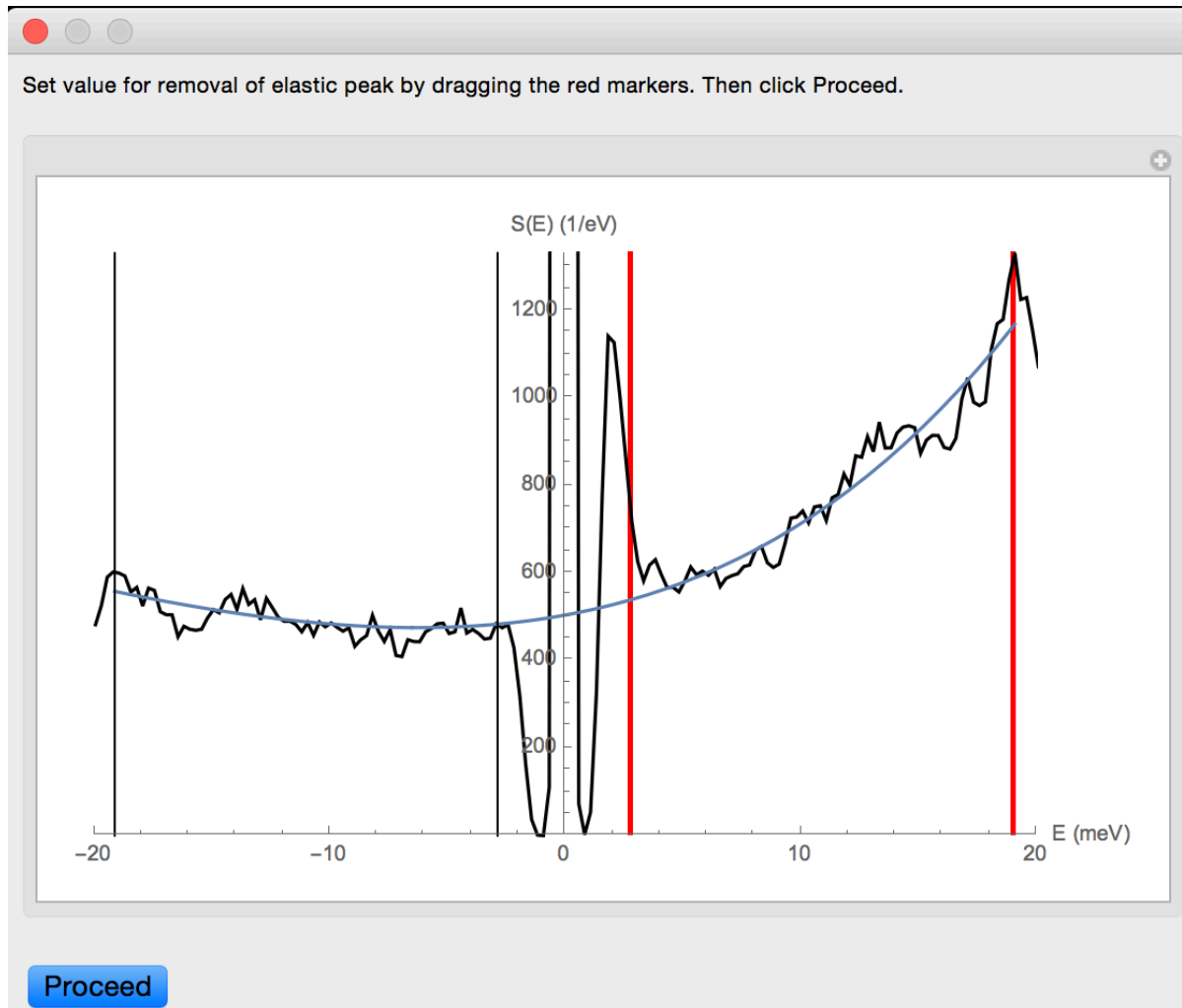
Elastic peak removal



No peak deconvolution



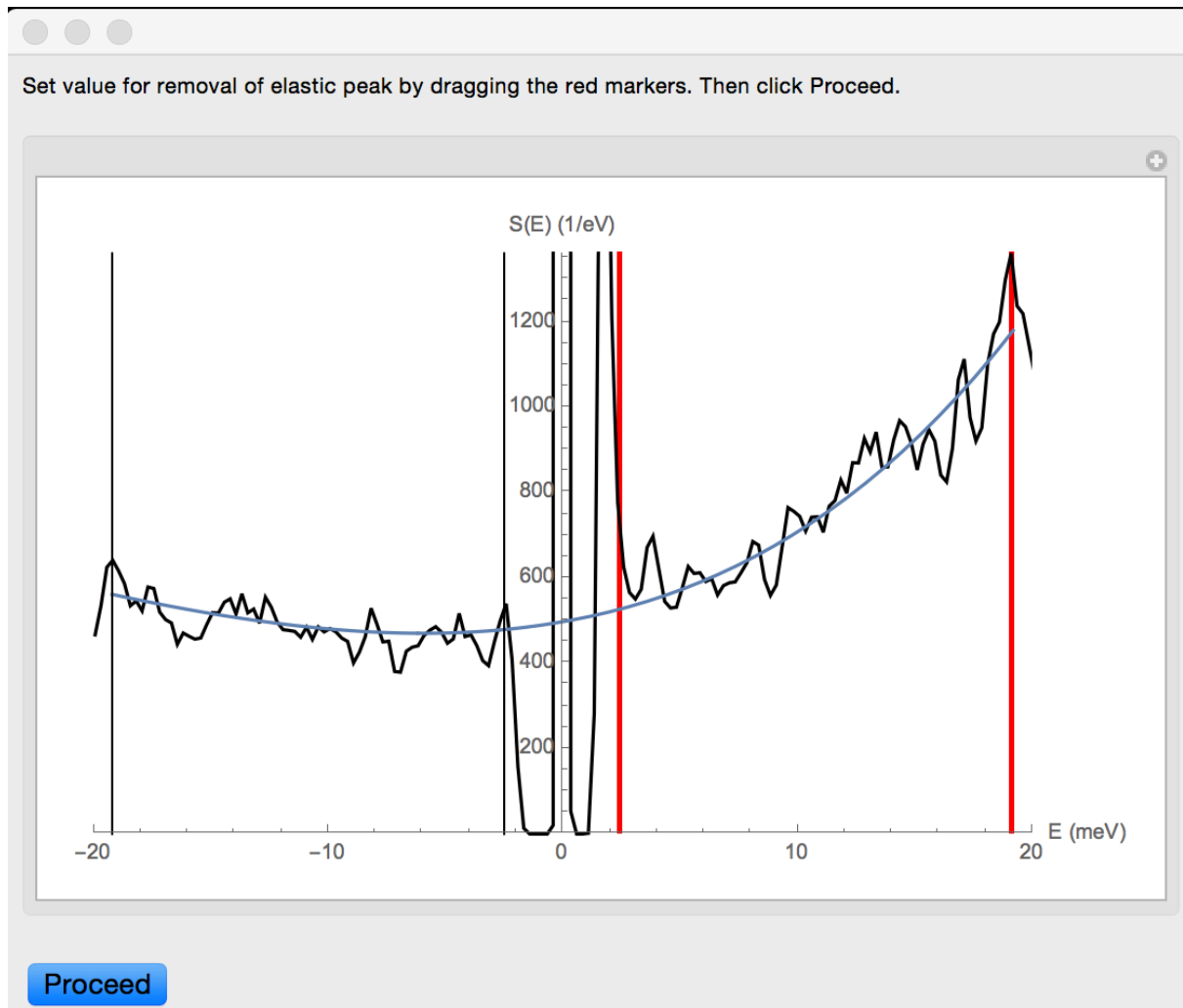
Elastic peak removal



10 iterations



Elastic peak removal



1000 iterations

Truncation and baseline definition

SciPhon 1.0

Select isotope: Fe-57

1. Load data file
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014/testpoubelle_Nov2014/Goethite_2014.dat

2. Load resolution file
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014/testpoubelle_Nov2014/Goethite_2014.res

3. Deconvolve resolution from data

4. Okay-proceed

Background subtraction (cts): 0
Experiment temperature in K: 300

5. Elastic peak removal

6. Energy truncation/baseline definition

7. Temperature calculation

8. Calculate DOS

9. Calculate sound velocities

10. Calc. Parameters 11. Export

Graphics output:

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

Proceed

Truncation and baseline definition

SciPhon 1.0

Select isotope: Fe-57

1. Load data file
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014_testpoubelle_Nov2014/Goethite_2014.dat

2. Load resolution file
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014_testpoubelle_Nov2014/Goethite_2014.res

3. Deconvolve resolution from data

4. Okay-proceed

Background subtraction (cts): 0
Experiment temperature in K: 300

5. Elastic peak removal

6. Energy truncation/baseline definition

7. Temperature calculation

8. Calculate DOS

9. Calculate sound velocities

10. Calc. Parameters 11. Export

Graphics output:

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

Proceed



Temperature determination

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

SciPhon 1.0

Select isotope:

1. Load data file
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014
testpoubelle_Nov2014/Goethite_2014.dat

2. Load resolution file
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014
testpoubelle_Nov2014/Goethite_2014.res

3. Deconvolve resolution from data

4. Okay-proceed

Background subtraction (cts):

Experiment temperature in K:

5. Elastic peak removal

6. Energy truncation/baseline definition

7. Temperature calculation

8. Calculate DOS

9. Calculate sound velocities

10. Calc. Parameters

11. Export

Abort/New session

References

Graphics output:

1 2 3 4

• Raw data
— Data Cst Bgd removed + Deconvoluted + Elastic peak and Baseline Removed + Trunc

Calculated T

Chi-Squared: Calculated temp:

OK



DOS calculation

SciPhon 1.0

Select isotope: Fe-57

1. Load data file
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014
testpoubelle_Nov2014/Goethite_2014.dat

2. Load resolution file
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014
testpoubelle_Nov2014/Goethite_2014.res

3. Deconvolve resolution from data

Background subtraction (cts): 0

Experiment temperature in K: 300

4. Okay-proceed

5. Elastic peak removal

6. Energy truncation/baseline definition

7. Temperature calculation

8. Calculate DOS

9. Calculate sound velocities

10. Calc. Parameters 11. Export

Abort/New session

References

Graphics output:

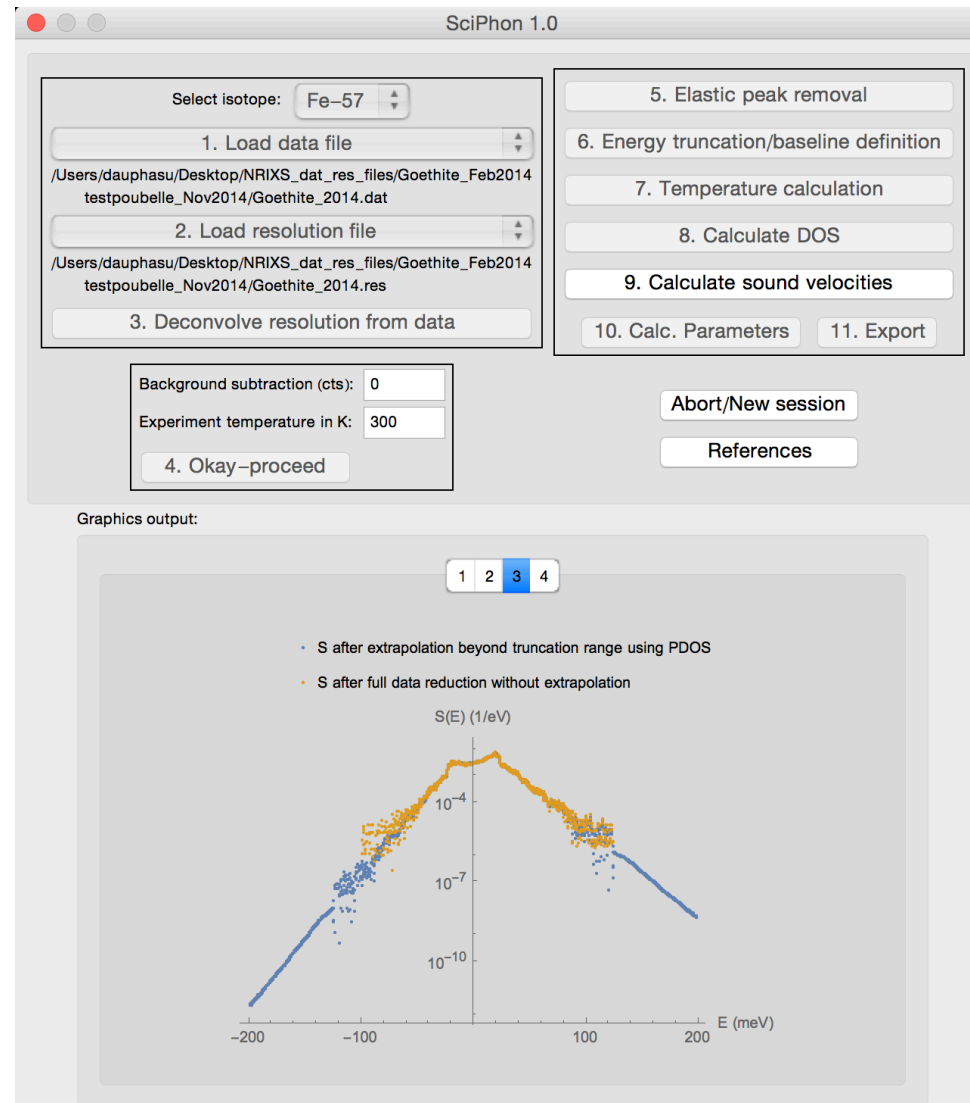
1 2 3 4

g(E) DOS (1/meV)

E (meV)



Extrapolation beyond the truncation range using the DOS





Calculate sound velocities

SciPhon 1.0

Select isotope: Fe-57

1. Load data file
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014
testpoubelle_Nov2014/Goethite_2014.dat

2. Load resolution file
/Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014
testpoubelle_Nov2014/Goethite_2014.res

3. Deconvolve resolution from data

Background subtraction (cts): 0
Experiment temperature in K: 300
4. Okay-proceed

5. Elastic peak removal
6. Energy truncation/baseline definition
7. Temperature calculation
8. Calculate DOS
9. Calculate sound velocities
10. Calc. Parameters 11. Export

Abort/New session
References

Density ρ of the material in g/cm³
4.27

Uncertainty (95 % ci) on ρ in g/cm³
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.

Graphics output:

1 2 3 4

- S after extrapolation beyond truncation range using PDOS
- S after full data reduction without extrapolation

$S(E)$ (1/eV)

E (meV)

Vd	Vp	Vs
3790	6384	3392
45	30	43

$g(E)/E^2$ (meV⁻³)

E (meV)

Proceed



Calculated parameters

SciPhon 1.0

Select isotope: **Fe-57**

1. Load data file

2. Load resolution file

3. Deconvolve resolution from data

Background subtraction (cts):

Experiment temperature in K:

4. Okay-proceed

Graphics output:

5. Elastic peak removal

6. Energy truncation/baseline

7. Temperature calculation

8. Calculate DOS

9. Calculate sound velocities

10. Calc. Parameters 11

Abort/New session

References

SciPhon v.1.0, Nicolas Dauphas, November 3, 2014

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

/Users/dauphas/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 × 10⁹ ± 6.76533 × 10⁸

A3: 1.11482 × 10¹⁴ ± 2.4666 × 10¹³

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 × 10⁹

A3: 1.1304 × 10¹⁴

-----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

The screenshot displays the SciPhon 1.0 software interface. The main window contains a workflow for data processing, starting with 'Select isotope: Fe-57'. The steps are: 1. Load data file (path: /Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014_testpoubelle_Nov2014/Goethite_2014.dat), 2. Load resolution file (path: /Users/dauphasu/Desktop/NRIXS_dat_res_files/Goethite_Feb2014_testpoubelle_Nov2014/Goethite_2014.res), 3. Deconvolve resolution from data, 4. Okay-proceed (with input fields for Background subtraction (cts): 0 and Experiment temperature in K: 300), 5. Elastic peak removal, 6. Energy truncation/baseline definition, 7. Temperature calculation, 8. Calculate DOS, 9. Calculate sound velocities, 10. Calc. Parameters, and 11. Export. There are buttons for 'Abort/New session' and 'References'.

Below the main window is a 'Graphics output' window titled 'SciPhon:'. It contains the following references:

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.

At the bottom of the graphics output window, there is a plot of temperature T (K) with a scale from 0 to 100, showing a curve that rises from 0 to approximately 100 K.

Conclusions

NRIXS is a powerful tool in isotope geochemistry

Beware of the baseline in NRIXS

Use SciPhon and give us some feedback



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