

Obtaining General User Beamtime and Guidelines for XAFS Manuscripts

Bruce Ravel¹ and Matthew Newville²

¹Synchrotron Methods Group, Ceramics Division
National Institute of Standards and Technology

²The Consortium for Advanced Radiation Sources
University of Chicago

APS XAFS Summer School
6-10 July, 2009

General User Access to the APS



GUPS & Papers

Ravel, Newville

Writing General User
Proposals

Writing XAFS
Manuscripts

Conclusion

All APS beamlines give at least 25% of the beamtime for General Users, which is open access to any researcher:

- Beamtime allocated by peer-review and open competition.
- Designed to bring in new people, keep access open to all.
- General User Beamtime can go to “local experts”
- Many beamlines give more than 50% General User time

The APS has three run cycles per year, which are, approximately

- 1 Feb 1 to Apr 30
- 2 Jun 1 to Aug 30
- 3 Oct 1 to Dec 20

Proposals are due around the middle of the preceding run.

See the calendar at

http://www.aps.anl.gov/Users/Calendars/GUP_Calendar.htm

XAFS Beamlines at the APS



GUPS & Papers

Ravel, Newville

Writing General User
Proposals

Writing XAFS
Manuscripts

Conclusion

Beamline	% GUP	% XAFS	Notes
2-ID (XOR)	> 50%	1/4	x-ray microprobe, XANES
4-ID (XOR)	> 50%	1/2	XMCD, magnetic XAFS
5-BM (DNDCAT)	= 25%	1/2	catalysis, enviro
9-BM (XOR)	> 50%	all	can do S and Cl!
10-ID (MRCAT)	= 25%	most	Catalysis, enviro, actinides.
11-ID (XOR)	= 25%	some	time-resolved.
12-BM (XOR)	> 50%	most	Catalysis, enviro, actinides.
13-BM (GSECARS)	> 50%	1/4	geo / enviro
13-ID (GSECARS)	> 50%	1/4	x-ray microprobe, geo / enviro
18-ID (BioCAT)	= 25%	some	biological systems
20-BM (XOR/PNC)	> 50%	all	general purpose XAFS
20-ID (XOR/PNC)	> 50%	most	x-ray microprobe, geo / enviro, time-resolved.

CAT A beamline operated by a Contributing Access Team

XOR A beamline operated by the APS

Other North American Synchrotrons

Information about the user programs at other synchrotrons including available beamlines and instructions for applying for beamtime can be found at:

NSLS Upton, NY (Long Island) _____ 10 XAFS beamlines
<http://www.nsls.bnl.gov/users/access/>

SSRL Palo Alto, CA (Stanford Univ.) __ 13 XAFS beamlines
<http://www-ssrl.slac.stanford.edu/userresources/index.html>

ALS Berkeley, CA _____ 3 XAFS beamlines
<http://alsusweb.lbl.gov/>

CLS Saskatoon, SK, Canada _____ 3 XAFS beamlines
<http://www.lightsource.ca/uso/>

CAMD Baton Rouge, LA _____ 1 XAFS beamline
<http://www.camd.lsu.edu/forms.htm>



GUPS & Papers

Ravel, Newville

Writing General User
Proposals

Writing XAFS
Manuscripts

Conclusion

Proposal Contents



GUPS & Papers

Ravel, Newville

Writing General User
Proposals

Writing XAFS
Manuscripts

Conclusion

The bottom line

Will this experiment result in a publication?

At the APS, the proposals are rated by panels of volunteers who read 20-30 proposals at a time. (The workload varies by synchrotron, but assume your reader is over-worked.)

Key Points for Successful Beamtime Proposals:

- 2-3 pages: **Take the time to make it short**
- Describe the importance of your science in terms **any** scientist can understand
- Aim broadly, your proposal will be read by physicists, chemists, biologists, etc....
- Describe your experiment well. Include details of samples to be measured and of experimental setup if non-standard. Account for the time you request.
- Consult with a beamline scientist and/or your collaborators before submitting proposal.

Matt's hints on proposal writing

(Bruce agrees with all of them!)

- Describe the “Societal Impact” in the Abstract – they love this.
- Describe other measurements that have been made on these samples.
- Be specific and explicit about:
 - Element(s) and edge(s) to be studied
 - Concentrations of elements to be studied.
 - Transmission, fluorescence, multi-element detector
- Give literature references. (Don't attach your CV. Don't attach PDFs of published papers.)
- Say you've taken this or a similar class! (Really!)
- If you're a student or postdoc:
 - say so.
 - list yourself as Spokesperson, not your advisor.
 - write the proposal yourself, with help from advisor / senior students.
- If you've had some beamtime and “need a bit more time”, include a plot of any data collected so far.
- List a 2nd choice beamline.



GUPS & Papers

Ravel, Newville

Writing General User
Proposals

Writing XAFS
Manuscripts

Conclusion

APS proposal scoring, lifetime and aging



GUPS & Papers

Ravel, Newville

Writing General User
Proposals

Writing XAFS
Manuscripts

Conclusion

Proposal Scores 1 (best) to 5 (worst) — like golf!

Proposal Shifts number of 8-hour shifts for next run and up to 2 years (6 cycles)

- Average Score for XAFS Proposals: ≈ 2.2 .
- Proposals that don't get time "age up" by 0.2 each cycle for 2 cycles and recompute each cycle
- Proposals live for up to 2 years or until the allocated shifts are used
- To get beamtime in more than 1 run for a proposal, you make a "Beamtime Request" for time in later cycles - **not a new proposal**
- to continue work, you can copy-and-paste an old proposal to start a "new" proposal

Caution!

The aging systems at NSLS and other synchrotrons work differently. Check each synchrotron's web site for details.

After you've submitted a proposal



GUPS & Papers

Ravel, Newville

Writing General User
Proposals

Writing XAFS
Manuscripts

Conclusion

- Most beamlines are oversubscribed - many by $2\times$ to $3\times$.
oversubscription = (requested days) / (available days)
- It may take a run cycle to get beamtime.
- You may get less time than you ask for.



- **DON'T PANIC** – it will become easier.
- Once you are in the system, everyone involved wants you to succeed (i.e. publish!).
- Most of these hints work for getting beamtime at other facilities and for other techniques.

The bottom line for manuscript writing



GUPS & Papers

Ravel, Newville

Writing General User
Proposals

Writing XAFS
Manuscripts

Conclusion

Write good science.

Don't write bad science.

Standards and criteria



GUPS & Papers

Ravel, Newville

Writing General User
Proposals

Writing XAFS
Manuscripts

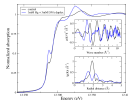
Conclusion

- 1 First report of S&C committee: Lytle, Sayers, and Stern (1988), Physica B, vol. 158, pp. 701-722
- 2 1993 and 2000 Reports from IXAS:
http://www.i-x-s.org/OLD/subcommittee_reports/sc/
- 3 Commentary by N.A. Young and A.J. Dent, J. Synchrotron Rad. (1999). 6, 799
- 4 Free-form wiki pages at XAFS.org:
http://xafs.org/Reporting_EXAFS_Analysis and
http://xafs.org/Common_Mistakes

The gospel of XAFS according to Bruce

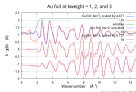
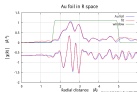
The eight beatitudes

- 1 Explain how you prepared your sample. Say what detectors you used. Explain or cite the beamline optics.
- 2 Cite your theory and analysis software.
- 3 Present theory in a way that it can be directly compared to data – preferably over-plotted, or at least stacked in a single plot.
- 4 Show data in energy, k , and R .



Try this if pressed for space:

- 5 Show or tabulate the principle background removal parameters, the FT and fit ranges, k -weight(s). Explain constraints and restraints.
- 6 Report uncertainties as determined from the fit.
- 7 Show the EXAFS fit many ways.



- 8 Be honest about the limits of what XAFS can measure.



GUPS & Papers

Ravel, Newville

Writing General User
Proposals

Writing XAFS
Manuscripts

Conclusion

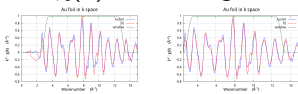
The gospel of XAFS according to Bruce

The four woes

- 1 Reporting uncertainties determined from the fit is better than implied uncertainties

e.g. “Uncertainties in ΔR are ± 0.01 ” in a table caption.

- 2 A plot of $\chi(k)$ not starting at 0 on the x-axis.



- 3 Incorrect or absent units on the y-axis of a plot of χ .

e.g. k^2 -weighted $\chi(k)$ has units of \AA^{-2} , its FT has units of \AA^{-3}

- 4 $\tilde{\chi}(R)$, the FT of $\chi(k)$, is **NOT** a radial distribution function (nor a pseudo-radial distribution function, nor a pair distribution function) and must never be referred to as such.

Bonus woe!

Replot your data with a real plotting program. Don't publish those crappy PGPLOT things from Athena or Artemis.



GUPS & Papers

Ravel, Newville

Writing General User
Proposals

Writing XAFS
Manuscripts

Conclusion

The grey areas

Like all good moral issues, some things are ambiguous.

“XAFS Debye-Waller factor” In XAFS, σ^2 is a mean square deviation in path length. In diffraction, $\langle u^2 \rangle$ measures the mean-square disorder in the distribution of atomic displacements from a lattice point. $\exp(-2k^2\sigma^2)$ might reasonably be called an XAFS DWF, but that obscures the important difference between σ_{XAFS}^2 and $\langle u^2 \rangle_{XRD}$

Letters journals Space is limited – it may not be possible, for example, to show data in more than one space.

Supplemental materials Use them! There is no practical limit to how many details you can present in the supplemental.

Sloppy terminology Some members of the XAFS community get worked up over jargon, for instance “self-absorption” or “pre-edge peak”.



GUPS & Papers

Ravel, Newville

Writing General User
Proposals

Writing XAFS
Manuscripts

Conclusion

Help yourself by making your reader happy!



GUPS & Papers

Ravel, Newville

Writing General User
Proposals

Writing XAFS
Manuscripts

Conclusion

The people who have been standing at the front of the room all week are likely at some point to rate one of your proposals or referee one of your articles.