◁研究会報告▷

第6回X線吸収スペクトル(XAFS)国際会議報告

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会議は1990年8月5日から11日まで英国ヨーク大学で開催された。この会議はもともとダレズベリー研究所で1981年に開かれたワークショップが発端となっている。これまでの会議を振り返ってみると，1983年のイタリア（フラスカテイ）の会議からEXAFSと吸収端微細構造に関する国際会議を名乗るようになり，翌1984年，米国スタンフォード，1986年フランス（フォテドヴロード）と続き，1988年米国シアトルでの会議から，EXAFSと吸収端微細構造(XANES)を総称してXAFS国際会議と呼ばれるようになった。ダレズベリーでのワークショップを含めると，今回が6回目にあたる。会議は大別して，EXAFSの理論や解析法を中心とする基礎，生物，物質科学，表面および界面，実験技術における応用の計5部門からなる。参加者は28ケ国から260名あまりで，発表件数は280件であった。会議の規模はフランスでの会議（論文数400）以来，それほど増えていないと記憶しているが，日本からの参加者は毎回増大する傾向にあり，今回の参加者は約40名であった。会議はレビューを中心とする総括講演，招待講演，口頭発表による2つのパラレルセッション，ポスターセッションと国際標準化のための特別セッションからなる。日本からの招待講演および口頭講演は8件で，ほぼ参加数に比例した妥当な数であるといえるが，筆者は1984年の会議から比べると格段に増えた印象をもった。論文は単行本として発行される予定であるので，詳細についてはそちらを参考にしていただきたい。以下に各セッションの概要といくつかの話題について報告する。なお次回は1992年に日本（神戸市）で開催されることがすでに決まっている。

1.XAFSの基礎

会議の冒頭でのレビューで，Pendryは，EXAFSの発展がシンクロトロン放射光と簡潔明解な解析法の発展によることを強調した。事実この会議自身，各国の放射光施設が中心となって開催されてきており，1983年の第2回会議以来，組織委員にはBienenstock(SSRL所長）やHaensel(ESRF所長）等が名を連ねている。この2人は今回も元気な顔をみせた。PendryはXAFSの本質である光電子の干渉を利用した新しい表面の構造研究手法として，表面のホログラムやSTMへのEXAFSの応用の可能性について講演した。理論面では，Natoliが吸収スペクトルにおける多体効果の影響が多重散乱理論に，配置間相互作用を取り入れることによって説明できることを示した。吸収端近傍の微細構造をより定量的に理解するには，ますます光電子放出の動的過程を記述する理論の発展が望まれる。またRehrはEXAFS理論の弱点ともいうべき非弾性散乱過程の取り扱いについて講演した。内殻励起における非弾性散乱は吸収スペクトルに大きな影響を与える。自己エネルギーをHedin−Lundqvistポテンシャルを用いて計算するΔSCF法によって，光電子の伝播過程

での非弾性散乱過程を，また光電子放出によってできる内殻正孔の緩和は多電子励起過程をグリーン関数で記述できることを示した。このうち，後者についてはより厳密なFujikawa,Hedin等による取り扱いが，藤川によって発表された。今回の会議では，前回シアトルで話題になった，曲面波による理論計算については，全く議論がなかった。このことは，曲面波の利用が普及したことを意味しているが，実験と比較した系統的な研究があってもよいのではないだろうか。

2．生体系

K.O.Hodgsonは生体系のXAFS研究のレビューを行った。彼もまたこの分野の発展が，放射光と高感度な蛍光検出法の利用に支えられていることを強調した。これまでの活性中心の金属原子に関する硬X線領域の研究に加えて，最近では軟X線領域に吸収端を持つ配位原子(S,Cl)も対象とするにいたった。これにはアンジュレーターの高輝度ビーム利用が重要な役割を果たしている。まだ波長固定のままの測定で，吸収端近傍の測定に限られているが，将来は挿入光源の波長を分光器と同期走査することにより，EXAFS測定が可能であろう。またX線回折による構造解析が結晶状態の平均構造を与えるという二重の意味でXAFSと相補的であることも広く認識されるようになり，両者を併用してより完全な構造情報を得ようとする方向にある。Lindleyはさらに生理現象の本質である化学反応の動的過程の研究の重要性を強調した。これには安定な放射光と各種時間分解測定手法の利用が必要となるが，今後の展開が最も期待される分野のひとつではないだろうか。蛍光検出法の高感度化のための半導体多素子検出器の開発は生体系に限らず重要な課題である。Cramerは半導体多素子検出器に関するレビューを行い，エネルギー分解能に重点を置く純Ge,Si(Li)の多素子検出器の現状と将来の高密度多素子ｉ検出器の可能性を報告した。楠等のMn光分解酵素に関する講演は半導体検出器により精度の高い吸収スペクトルが得られることを示すものとして注目された。ポスター発表全般を振り返ってみると，今回の会議では吸収端近傍(XANES)の応用が目立っており，EXAFSの発表件数が減っていることは気がかりではあるが，生物物理と放射光に関する会議は逆の方向にあるのでこれでよいのかも知れない。

3．物質科学

Lengelerは物質科学への応用に関するレビューを行い，最近のトピックスとして，超伝導酸化物，Frahm等による迅速測定法，全反射を用いた表面研究の成果を報告した。今回の会議では特に超伝導酸化物のセッションは設けられなかったが，超伝導転移付近の熱振動の温度依存性の異常や酸素効果に興味が集まっていた。超伝導酸化物に関する口頭発表は筆者等のNd−Ce−Cu−O系の酸素効果に関するものだけで，できれば前回のように独立したセッションを設けて欲しい気がする。特に温度依存の異常なふるまいについては解析法の問題等を含めて議論する機会が必要であろう。触媒に関連した応用はEvans,Koningsberger等によるレビューがあり，反応過程でのその場観察の重要性が示された。特に後者の講演では金属一配位間の中距離相互作用の存在が示されたが，これは精密な測定および解析の進歩による所が大きい。精密実験のための安定な放射光と光学系，特に結晶分光器への関心は次第に高まっている。そのほか，口頭講演としてAbruhaにより電解反応の固液界面のその場観察への全反射の利用，北野により結晶欠陥における金属析出，SadocによりAlCuFe準結晶への応用がそれぞれ報告された。Lagardeは軟X線領域の吸収スペクトルについてレビューを行い，多重散乱理論による解析によって立体配位構造や電子状態に関する情報が得られることを示した後に，希土類金属クラタスーへの応用を紹介した。クラスターの電

子状態および微視的構造を調べる試みは筆者の知る限りこれが初めてであるが，硬X線領域においても今後の発展が楽しみな研究分野のひとつであろう。

4．表面，界面

Setteは軟X線領域の円偏光アンジュレーターとドラゴン分光器を用いたビームラインとそれを用いた強磁性体の円偏光二色性に関する講演を行った。輝度と分解能を兼ね備えた新しい軟X線分光器であるドラゴンは，その特徴を生かして超伝導酸化物の酸素の吸収スペクトルについても質のよいデータを提供している。これら軟X線領域での磁性体の電子状態の研究は先駆的な試みであるが，硬X線領域での研究はすでに各国の放射光施設で開始されており，今回もSchutzがフェルミ面のd電子状態について実験と理論の比較を行い，1電子理論によって実験がほぼ説明できることを示している。筆者は硬X線領域の表面XAFSが全反射と半導体検出器の組み合せで可能であることを示し，Si/Ge超格子の研究を報告した。この手法は高輝度ビームの利用や検出効率の改良の余地があり，現在開発中のマルチポールウイグラーラインと多素子検出器により，将来表面研究の強力な推進力となるものと考えられる。Stohrは吸着種を原子と分子に分けて，それぞれの3次元配位構造の研究手法を中心に，軟X線領域の表面XAFSのレビューを行い，太田はS,Cl/Ni系を例に定在波の併用による表面吸着サイトの詳細な研究を紹介した。またGreavesは全反射下での蛍光検出法および反射率による硬X線領域の表面，界面研究を紹介したが，方法論を実証する迫力ある実験結果は見あたらなかった。ポスター発表にも興味ある成果が多かったが，一方では取り消しの発表もまた多かったのは，この分野の実験効率がよくないことによるのだろうか。

5．実験技術

Lytleは実験技術の進展に関するレビューを行い，種々の新技術（半導体多素子検出器による高感度化，分光器の連続走査による高速化等）を紹介した。分光器を中心とする光学系は次第に精度を要求されつつあるが，高輝度ビームの利用では分光結晶の熱負荷が与える問題について議論する機会がなかったことは残念である。Fontaineはエネルギー分散法の現状を紹介したが，特に生体反応など，希薄な系での動的過程の研究に適用する上で，光源の安定性が重要であることを強調した。Frahmは分光器走査に同期した連続型のデータ収集法によって，高速測定が可能であることを示した。この方法はエネルギー分散法と異なり，蛍光検出法にも使用できる点は魅力的であるが，分光器のエネルギーと回転角度の厳密な対応関係が要求される。この点に関してはまだ議論の余地が多いように思えた。宇田川は実験室測定装置の現状をレビューしたほか，新しい実験技術として，田路がX線ラマン法をまた升島が光音響法を紹介し注目を集めた。今後これらの手法が実用的手法となるためにはらさに高輝度ビームを利用することが必要であり，将来の高輝度放射光の利用が望まれる分野である。GoulonはESRFのXAFSビームライン計画を紹介した。新しい偏光ウイグラーを利用した直線偏光および円偏光の実験およびエネルギー分散法のための二つのビームラインが計画されており，これらは1994年に予定されている最初の実験に向けて準備されつつある。チューブナルX線アンジュレーターの利用によってXAFSの画期的な展開が期待できる。ESRF，APSともにまだ具体的な計画がないので，これらについては是非ともわが国で先鞭をつけたいと思うが，分光器の熱負荷等この分野に共通した技術開発を積極的な国際協力によって推進したいとの意見を持つ研究者が多く，放射光も国際協力の時代に入ったことを認識させられた。

6．国際標準

理論，実験，解析，データベースの4部門についての国際標準化の試みは1988年に最初の国際ワークショップがNSLSで開かれ，ついでシアトルの会議でその報告書が承認されて以来順調に進みつつある。この会議では第2回目のワークショップの結果が報告されたほか，これまで国際会議ごとに組織されてきた国際委員会(International Advisory Committee)を国際会議運営とは別の恒久的な組織(Standing Committee)として存続させ，標準化のための国際ワークショップを含む各種ワークショップ開催の企画，運営にあたることになった。この組織はStern,Garner,筆者をそれぞれ正，副委員長および幹事とする暫定的なワーキンググループで規則等が検討され，黒田教授を委員長とする次回神戸での会議で正式に発足することとなった。

今回の会議は相互に関連が少ない分野をパラレルセッションにするなどプログラム編成にかなり工夫されているが，それでも会議が終わってみるとポスターを含めて，ききのがした発表が少なくない。2年毎の開催ということもあって，残念ながらシアトルの会議から画期的な展開がみられた分野はさほど多くなかった。ますます高精度な実験が行われ詳細な議論が行われるようになってきており，着実な進歩を遂げているといえよう。一方，将来の研究の方向性として動的過程の研究は生体，物質科学，表面の各分野で重要を位置を占めるであろう。今回の会議では第2世代の蓄積リングを使っての信頼できる質の高いデータが数多く発表され，研究成果を左右する光源の性能の重要性があらためて認識された。また，挿入光源を有効に利用するには測定技術側，特に光学素子の熱負荷の問題や高効率検出器の開発が重要で，この点に関しては1992年の会議のあとで開かれる高輝度光源の利用技術に関するワークショップで実りある議論が行われるものと思う。今回の会議は城壁で囲まれた古都ヨークで開催された。会議の期間中ヨーロッパは記録的な猛暑に見舞われ，パブで飲むビールが楽しみな毎日であった。ところで筆者は英国に特別の思い出がある。1978年夏，大学院生の頃，エジンバラのアモルファス半導体国際会議の帰り路，ヒースロー空港で偶然Sayersに会ったのがXAFSとの出会いであった。その後シアトルからNorth Carolinaに移ったばかりの彼を訪ねてから12年が経過した。再会を喜びあってグラスを傾けると物性研当時の古いX線発生装置が懐かしく思い出された。苦しい経験であったが今では妙に懐かしいのは何故だろうか。その後筆者がエジンバラに向けて12年前と同じFlying Scotsmanに乗り込んでヨークをあとにしたことは言うまでもない。

Report on International Workshops on Standards and Criteria in XAFS

Introduction

The field of XAFS spectroscopy has grown dramatically over the last two decades and has significantly matured. Improvements in experimental methods, as well as refinements to the theory and data analysis, have greatly improved the range and reliability of the technique. In

spite of these successes, however, the average technical quality of papers based on XAFS remains disappointingly low. Part of this is attributable to a relative paucity of generally accepted textbooks on the subject, and a lack of written, comprehensive, generally accepted, standard procedures for the practice of XAFS. New practitioners of the technique often must learn important lessons the hard way, or sometimes never learn them at all. Even experienced scientists sometimes have significant gaps in their understanding of the issues. Consequently, the average competence of referees of XAFS papers is variable, further contributing to the problem. This situation, apart from being very inefficient, has harmed the credibility of the XAFS literature as a whole.

The International Workshops on Standards and Criteria in XAFS (X-ray Absorption Fine Structure) represent an attempt to help rectify these problems. The first workshop was held March 7-9 1988, and a written report, after ratification by the International Advisory Committee and the delegates of the Vth XAFS conference, was published in Physica B158 (1989) 701-722. Since then workshops have been held at Jaipur (11-22 December 1989) and Brookhaven (19-20 May 1990). The workshop at Jaipur particularly discussed the issues concerning Laboratory XAFS and some aspects of theory. The Brookhaven workshop considered all of the issues raised in the original 1988 workshop but also discussed the question of Education and dissemination.

The following document is a summary report of these workshops, which is to be published in the Proceedings of the Sixth International Conference on XAFS, after ratification by the IAC and the delegates of XAFS VI, York, England, 1990.

This report has been primarily prepared by the group leaders of various sub-groups of the workshops. The Brookhaven report was compiled and edited by Grant Bunker and the Jaipur report was compiled by Samar Hasnain, who was also responsible for the final form of the combined report in whcih he was assisted by Dale Sayers.

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Subgroup Report: Theory of XAFS

Brookhaven
Group Leaders: John Rehr, Steve Gurman
Participants: J. Mustre de Leon, T. Tyson

Jaipur
Group Leaders: Reno Natoli, Steve Gurman
Participants: Workshop delegates

The theory of XAFS has recently undergone extensive developments. During the two years since the 1988 EXAFS workshop report many formal developments have been incorporated into *ab*

initio codes and tested against experiment. As a consequence, there is now general agreement on the minimal requirements of the theory. Two levels of theoretical description were identified in the previous workshop report, one based on tabulated phases and scattering amplitudes and the other based on *ab initio* codes. Because of advances in accuracy and computational speed, the use of one of the currently available codes (EXCURV, FEFF, Frascati) is now preferable to tables when a suitable workstation is available. Tabulated standards are still useful, but they are presently incomplete. We recommend that tabulations of mean free paths and many body reduction factors should also be made available.

We now summarize the current theoretical status of XAFS. It is convenient to separate the theoretical description into several parts: a) propagation of the photoelectron and scattering by atomic potentials; b) the calculation of the scattering potential; and c) Debye-Waller and other many-body reduction factors.

I. Theory of EXAFS

a) Scattering theory

The formal problem of propagation and scattering of the photoelectron is generally regarded as solved. Multiple scattering contributions may be included using the small atom or separable approximations (S.J. Gurman *J. Phys. C* , 3699 (1988); J.J. Rehr and R.C. Albers, *Phys. Rev B.* **41**, 8139 1990)) or the more accurate spherical wave expansions (S. J. Gurman, *et al., J. Phys. C* **17**, 143 (1984); J.J. Rehr *et al., Phys. Rev. B* **34**, 4350 (1986)). The errors in the plane wave formulation are sufficiently large that its use in quantitative comparisons is incorrect. The convergence of the spherical wave theory may be checked by comparing with the exact, but slow curved wave theory (R. W. Strange *et al., J. Amer. Chem. Soc.* **109**, 7157 (1988)) or by using the "spectral radius criterion suggested by the Frascati group (i.e., the largest eigenvalue of G_t being less than unity); as a rough estimate, the multiple scattering expansion will fail to converge when $|f(0)/R| \geq 1$. However, this is a conservative estimate, since large angle paths do lead to smaller contributions than forward scattering ones. Special care must be taken in dealing with absorption by polarized x-rays, as the effective curved wave back-scattering amplitudes are polarization dependent. This difference should be recognized and incorporated in existing codes. Theories which include polarization effects have been developed for both single scattering (J. J. Barton *et al., Phys. Rev. B* **34**, 2207 (1986); J. Mustre de Leon *et al., Phys. Rev. B* **39**, 5632 (1989); S. J. Gurman *J. Phys. C* **21**, 3699 (1988)) and multiple scattering (M. Benfatto *et al., Phys. Rev. B* **39**, 1936 (1989)). The general multiple scattering theory developed by Natoli et. al., which was extensively described at the Jaipur workshop, could be of much use fot energies below 100eV where many multiple scattering paths may contribute. Also the development of a multi-channel MS theory by Natoli et. al. incorporates into the theory the dynamical excitations of the atom, usually referred to as shake up and shake off and treated as an empirical parameter (see next section).

b) Scattering Potentials

The calculation of reliable scattering phase shifts requires the use of potentials that incorporate molecular and many-body effects. Adequate Coulomb potentials away from the edge region may be generated by using the Mattheiss prescription of overlapping atomic charge densities from self consistent Dirac atom calculations. The use of relativistic atom densities is particularly important for the case of heavy elements. Exchange-correlation contributions should be calculated using an energy dependent potential.The Hedin-Lundqvist potential seems to be adequate giving better phases than the Dirac-Hara potential plus a phenomenological imaginary part (J.J. Rehr *et al., Physica B* 158, 417 (1989). The use of ground state exchange-correlation potentials, e.g., the X_α potential, leads to significant errors in distance determinations (.02-.03 Å), and should now be avoided (J. Mustre de Leon, *Ph. D. thesis, University of Washington* (1989)). When comparing with experiment, core-hole lifetimes and monochromator resolution (see Data Analysis section in this report) should also be taken into account. The absorbing atom should be calculated with a neutral, relaxed core-hole configuration, again using a Dirac self-consistent atom calculation. We recommend that the energy reference, E_0 be left as an adjustable parameter due to the difficulty of calculating the Fermi energy in arbitrary systems, and the fact that most theoretical potentials are not fully self-consistent. However, it should be checked that the variation of E_0 is within physically reasonable limits. Many body amplitude factors may be

calculable in the future (see, e.g., D. Lu and J. J. Rehr, Phys. Rev. B 37, 6126 (1988)); however, at this point in time we recommend the use of an overall adjustable amplitude reduction factor S_0^2 which is allowed to vary within physical limits, e.g. about 0.7-1.0.

c) Debye-Waller factors

We feel that the use of the harmonic approximation is one of the weakest points in the XAFS calculation; it should only be relied on when thermal and structural disorder is known to be small. For multiple scattering paths the plane wave form $\sigma^2(1-\cos(\theta))$, where θ is the scattering angle, is often sufficiently accurate for practical use. We recommend that non-perturbative approaches to highly anharmonic cases should be explored (inverse Monte Carlo, [S. J. Gurman, to appear in J. Phys. C.], or direct fit to the radial distribution function [J. Mustre de Leon et al., in XAFS VI proceedings] in future work.

d) Comparison of Theory and Experiment

Quantitative comparisons of different theoretical formulations with expriment should be carried out. The preliminary findings of such comparisons for several materials [D. C. Koningsberger et al., unpublished] are reflected in the above recomendations. The difference between different codes resides in the potential used. Other, more extensive, comparisons are essential.

II. Theory of XANES

Ab initio computation of the XANES spectra has been handicapped by a lack of computational schemes based on accurate molecular potentials. Consequently, only qualitative interpretations of the features seen was possible. However, two models are now being developed that are making quantitative comparisons between theory and experiment possible. These approaches not only yield accurate energy spacings (which already was possible using muffin-tin (MT) potentials [Kutzler *et al., J. Chem. Phys.*73, 3284 (1980)] but are approaching accurate amplitude reproduction. Both methods are based on nonmuffin-tin potentials. The method of Ellis [D. Guo *et al.*, Phys. Rev. B **41**, 82 (1990)] goes beyond the MT approach by making use of the discrete variational method based on numerical atomic basis functions. Cross sections are computed using these accurate potentials in the bound state regions and using the MT approximation hem in the continuum region. The method has been used to simulate the spectra of copper oxides. The second approach is based on the non-MT theory of C.R. Natoli *et al.*, [*Phys. Rev. A* **34**, 4682 (1986)]. In this method full potentials are obtained by including nonspherical terms of the potential function expansion in the atomic, outer sphere and interstitial regions. Foulis has refined the theory and implemented it as a set of computer programs [D. L. Foulis et al., J. Phys. (Paris) C 8, 597 (1985); D. L. Foulis, Ph. D. Thesis, University of Warwick, 1988]. The full potentials are used to calculate both the bound state and continuum region cross sections. Tests on molecules are currently in progress but results seem promising. Some of the problems of the XANES region which still have to be addressed are related to the neglect of many body corrections which are particularly important near the edge. The full MS theory developed by Natoli et. al. show that at low energies the MS expansion does not converge so that a cluster calculation involving matrix inversion, such as the Pendry-Durham (for a recent example see Strange et. al. JACS, 112,4265-4268(1990)) code is essential.

Subgroup Report: Data Analysis

Group Leaders: Grant Bunker, Daryl Crozier
Participants: Norman Binsted, Yanjun Ma, Alex McKale, Ed Stern, Marius Vaarkamp, Ke Zhang

The discussion of the data analysis group focussed on the quality of data analysis and its presentation in published papers, procedures for the estimation of errors, and the reliability of structural information obtained for second and higher shells.

The 1988 Workshop concluded that the basic principles and procedures of data analysis are well understood, but that this was not yet reflected in the majority of published papers. Since 1988 there has been only limited improvement in the quality of the literature. Thus the data analysis group agreed that more forceful action is necessary. It recommends that all published papers satisfy a minimum set of requirements and that the referees of EXAFS papers enforce them. A suggestion for the minimum requirements is given at the end of this section for discussion and implementation at the XAFS VI International Conference. Also provided is a supplementary list of suggestions that would contribute to the information content of published papers.

Estimation of Errors

The assessment of errors associated with structural parameters deduced from EXAFS remains an important problem. It is complicated by the requirement to include non-statistical errors in the estimate in a systematic way. This question was discussed at length in the 1988 Workshop Report where it was encouraged that experience be gained in evaluating errors using a functional of the generic form of eqn. [1] defined below. A subcommittee is suggested to the IAC consisting of Norman Binsted and Samar Hasnain (Daresbury), Grant Bunker (Biostructures Institute) and Ed Stern (University of Washington). The committee will examine different ways of applying eqn. [1] and make recommendations within one year.

The Reliability of Second and Higher Shell Information

EXAFS is now a mature structural technique with a recognized ability to specify the average structural parameters of the first nearest neighbours. As reported in the 1988 Workshop Report, a simple test of the reliability of first shell analysis was conducted. Eleven different research groups received data for a reference system and an unknown, the identity of which was not revealed. The results of their different analysis of the unknown were very consistent: agreement was found to better than 0.02 Å maximum (0.01 Å standard deviation) for the nearest neighbour bond length and about 10% maximum (5% standard deviation) in the coordination number.

There are many areas where EXAFS can provide significant structural information for second and higher shells. But the analysis is normally complicated by a number of factors, some of which are: multiple scattering, difficulty in obtaining reference amplitudes and phase shifts with a consequent reliance upon theoretical calculations for both their angular and radial dependence, inelastic effects, the loss of information associated with a finite value of k_{min}, and greater contributions from anharmonicity and asymmetrical distribution functions. The committee's brief will be to extend the reliability tests to include second and higher shells.

It is agreed that the initial tests should involve systems where specific factors can be varied in a controlled way. For example, by applying pressure to ReO_3, the rhenium-oxygen octahedra are forced to rotate, changing the Re-O-Re forward scattering angle by a known amount and thus changing the contributions of multiple-scattering. We would like to receive additional suggestions for appropriate systems for analysis. We would also like to encourage different research groups to become involved in these tests.

Summarizing and Presenting Results

The committee suggests the following minimum requirements in the publication of papers:

1. Display raw data, preferably as $\chi(k)$ or $k\chi(k)$.
2. State clearly the numerical procedures used to remove the background and to normalize the data.
3. Identify the location of $k = 0$ relative to readily distinguishable features in $\mu(E)$ (or its derivative).
4. Describe window functions used in k-space and in R-space.
5. State window ranges (k_{min}, k_{max}; R_{min}, R_{max}).
6. In extracting structural parameters, if reference compounds are used state the crystallographic data (N,R) and cite the publication.
7. If theoretical amplitudes and phases are necessary, it is recommended that they be calculated in the spherical wave approximation. If the McKale tables are used, the

scattering amplitudes must be corrected for inelastic effects (see the theory section of this Workshop Report for recommendations). Seah and Dench provide a convenient parameterization of the mean free path for elements and inorganic compounds.

8. When comparing theoretical amplitudes with experimental data, corrections must be made for the monochromator resolution function and the energy dependence of the normalization function. The latter can be approximated using the McMaster Tables (as discussed in the 1988 Workshop Report, page 713). The former can be approximated by a Lorentzian or Gaussian broadening function.

9. Parameter error estimates should *always* be presented. The prescription used to estimate error bars should be described in detail.

10. The results of fitted data should be presented in such a way that it is clear that the number of fit parameters does not exceed the number of independent points, N_{pts}. As discussed in the 1988 Workshop Report

$$N_{pts} = 2\,\Delta k\,\Delta R/\pi$$

where $\Delta k = k_{max} - k_{min}$ is the k-space range of the data and $\Delta R = R_{max} - R_{min}$ is the width of the window in R-space.

This restriction on the number of data points applies even when the unfilterd $\chi(k)$ is fitted to a model (see footnote). The ΔR to be used is the same ΔR that one would have used if the data had been fourier filtered. This restriction occurs because the information content of the EXAFS interference function is bandwidth limited. In a filtered data, it should also be realized that Δk is limited by the useful range of the data: it must not be increased by extending k_{max} beyond the k value where the noise level exceeds the amplitude of the interference function.
In addition, as indicated in the 1988 report, the committee also offers the following suggestions to improve the information content of published papers:

1. Errors should be evaluated from a function of the generic form (which is similar to but not identical with the statistical χ^2 function):

$$\varepsilon_v^2 = (1/v)\ \sum_i^{Npts}(Data_i - Model_i)^2/\sigma_i^2, \qquad (1)$$

or its alternative form (see 1988 report),

$$\varepsilon_v^2 = (N_{pts}/v)(1/N)\ \sum_i^{N}(Data_i - Model_i)^2/\sigma_i^2. \qquad (2)$$

In [1] and [2] $v = N_{pts} - p$ where p is the number of fit parameters and σ_i^2 is the standard deviation of each data point i. In accordance with canonical least squares fitting theory, σ_i^2 must include statistical uncertainties in the data. In addition, at the 1988 workshop it was suggested that nonstatistical uncertainties also be included according to

$$\sigma^2 = \sigma^2_{statistical} + \sigma^2_{nonstatistical}$$

Footnote added by S. S. Hasnain: This restriction on the number of independent points does not apply when the unfiltered $\chi(k)$ is fitted to a model. In this case the number of independent points which define a typical EXAFS profile in a unit of k is far in excess of five points.The independence of data points should be worked out based on diffraction principle. The band pass effect is treated in the scattering theory by the use of the imaginary part of the potential, Vp^i.

Discussion of $\sigma^2_{nonstatistical}$ can be found in the 1988 Workshop Report (pages 709 to 712). This criterion is expected to give conservative estimates (perhaps too conservative) for the parameter errors. The latter proposal is currently under evaluation.
Three essential ingredients of equations [1] and [2] that should be born in mind are:

a) The experimental uncertainty σ_i in each data point as a function of k should be included. The alternative of estimating the average error from the best fit residuals is *not* recommended, because by doing so one assumes, in effect, that the hypothetical model used in the fit (e.g. number of shells, types of atoms) is *a priori* correct. The *data*, together with the experimental uncertainties

σ_i, should tell you whether the fit is good or not.

b) A "price" in ε_ν^2 must be paid for including more parameters in the fit. Enlarging the parameter space cannot make a fit worse (unless numerical instabilities occur). This is the importance of the $1/\nu$ prefactor in eqn [1]. If you add more parameters, at some point ε_ν^2 as defined in eqns [1] and [2] will stop decreasing, and even increase. If the factor $1/\nu$ were not included, the squared residuals would in general keep decreasing as more fit parameters are added.
c) The number of independent data points is reduced by fourier filtering, because the information contained in the r-space window is only a fraction of the total r-space.

2. Include the correlation matrix as a table to provide an indication of the correlation between fit parameters. Space restrictions will probably dictate that the correlation matrix be restricted to the single most significant structure.

3.Scale the ordinate axis on the modulus of the FFT (these are *not* arbitrary units). The numerical magnitude of the Fourier transform provides useful comparative information for the reader. We propose the following normalization convention: on the forward (k to r space) transform, multiply the data by the k grid spacing, and divide by $\sqrt{\pi}$. On the inverse transform multiply the data by the r grid spacing, and again divide by $\sqrt{\pi}$. This maps the discrete Fourier transform onto a continuous transform (exp(-i2kr) kernel) eliminating any dependence of the scale on the number of points used in the transform, the grid spacing, etc. The unit for the transform of k^n weighted $\chi(k)$ data then is $Å^{-(n+1)}$. Also, phases should be defined so that when a pure sine wave sin(2kR) is transformed, the imaginary part of the transform and the modulus should peak at the same r-value.
4. Several different data analysis packages are available for use by the general EXAFS community. Since these packages calculate amplitudes and phases using different assumptions and treat some aspects of analysis in different ways, if you use one you should state which one.

Subgroup Report: Experimental Methods

Group Leaders: J. Goulon, S. M. Heald
Participants C. Bouldin, A. Edwards, B. Hedman, K. Hodgson, K-Q Lu

In the past report the experimental group provided a detailed description of experimental issues and problems. We feel that this description remains timely. In the present report we concentrate on implementing solutions to the problems, and look towards the future. The major areas considered are the minimum requirements for reporting experimental data, deposition of data, general user support, continuing problem areas, and future directions of XAFS.

Minimum Requirements for Reporting Experimental Data

In order to improve the quality of published EXAFS papers it is suggested that the following standard information should be included in all papers about x-ray absorption measurements:

1) Where the sample was measured (X-ray source and experimental station).
2) Electron beam current and energy.
3) Type of monochromator, especially crystal type and cut.
4) Details of harmonic rejection system (mirror, detuning, etc).
5) Type of detectors used (energy resolution, dead time, harmonic sensitivity).
6) Energy resolution and calibration.
7) Sample preparation (particle size, checks for uniformity and phase purity).
8) Sample thickness, *both* μx and $\Delta\mu x$.

It is further recommended that the list given above should be distributed to referees and that papers that do not include this minimum information should not be published. In addition to this minimal list, if the paper makes quantitative use of other experimental parameters, such as degree of x-ray beam polarization, then *some* quantitative estimate of such parameters must be given.

As an example of how to present this minimum information, we demonstrate below that in most cases standard "boiler plate" can be used. Sample preparation details are clearly dependent on the particular experiment, but a specific example of the type of information needed is given below. Where it is possible to use standard text, the "variables" to be filled in are given in upper case and underlined:

"Samples were measured on BEAMLINE X23A2 at NSLS with an ELECTRON BEAM ENERGY OF 2.5 GEV and a MAXIMUM STORED CURRENT OF 200 MA. Data were collected with a FIXED EXIT MONOCHROMATOR using TWO FLAT SI (220) CRYSTALS. Harmonics were rejected by using a GRAZING INCIDENCE MIRROR. Data were collected in TRANSMISSION MODE using ION CHAMBERS with NITROGEN FILL GAS. Energy resolution was estimated to be ABOUT 3 EV by the CU FOIL 3D NEAR EDGE FEATURE. The ENERGY CALIBRATION was monitored using a REFERENCE SAMPLE AND A THIRD ION CHAMBER, and was set as 8980 EV AT THE CU 3D FEATURE.

Samples were prepared by powdering, sieving and then selecting small particles less than 10 microns in size by floating the powder. The particles were then deposited on tape. About 7 layers of tape were used to fabricate samples with $\Delta\mu x$ of 0.5 to 1.0 and total μx less than 1.5. Sample purity was determined by x-ray diffraction and maintained by use of ceramic grinding tools."

Deposition of XAFS data

Beyond the need to report a minimum requirement of experimental details, there is problem of reporting the actual data used in the publication. In some fields such as small molecule crystallography, virtually every reputable journal now requires deposition of structures factors for each structure published. In this case, however, the archival form of the deposition material is determined primarily by the particular journal (most commonly microfilm). As a practical point, the implementation of an internationally accessible XAFS data base offers an excellent opportunity for providing an easily accessible, standardized means for storage and retrieval of XAFS data. A more significant, and controversial point regards the question of specific recommendations as to when and what data should be deposited. On one hand, it is essential that when a scientific paper is published, the data necessary to validate the scientific results be made available. On the other hand, the scientist may wish to have time to carry out more complete analysis after a preliminary publication, and, thus, has the point of view that the data deposition should be delayed. There are also questions of disclosure of proprietary information. The issue of scientific data deposition is receiving both international as well as local attention, and the XAFS community would be wise to establish its own recommended policy, rather than wait for one to be dictated by other bodies. We recommend that this point be more widely discussed within the XAFS community as a whole.

General User Support

Initially many synchrotron radiation beamlines for XAFS were facility operated, and substantial support was provided for outside users. More recently the trend has been towards allowing interested groups (known as Participating Research Teams at NSLS) to construct and manage beamlines. This has the advantage of fostering innovation and broadening the funding base for beamline construction, but generally makes life more difficult for outside users who are not associated with a PRT. Each beamline is different and the levels of support provided for users is quite variable. It is our view that general user should not be slighted in the push to instrument new beamlines.

The XAFS field is different from many others in that it is largely synchrotron radiation based. Only limited opportunities exist for training outside of synchrotron radiation facilities. This means that the facilities will continually be hosting inexperienced users. For these users we feel that general user beam lines with associated support staff are necessary if the XAFS field is to continue to attract new users. Thus, we recommend that new facilities provide, maintain, and support general user facilities for XAFS studies in addition to PRT type beamlines. This policy has the additional advantage that a synergistic relationship is developed between staff scientists providing the support and the general users, benefitting both sides. The facility becomes more attuned to the needs and desires of one of its largest communities, and the users are afforded valuable training.

Continuing Problem Areas

The group identified three main problem areas for future work. These are related in that they all limit the quality of acquired data below that which would be predicted from statistical analysis of the photons available. The first of these is detectors. The general focus of our discussions was on detectors for fluorescence, although time resolved studies, surface XAFS, and soft x-ray experiments could benefit from improved detectors. The gains which can be realized from improved detectors are substantial. For example, the recently developed 13-channel solid state detector has dramatically improved the statistics of a number of experiments, but it is still a long way from collecting all of the available fluorescent x-rays. In general the technology exists (mainly derived from high energy physics efforts) to make improved detectors, but the development costs are generally too large for a single group to undertake.

The second area is the development of XAFS monochromators. The XAFS experiment is extremely dependent on monochromator quality, and the difficulties in designing good XAFS monochromators are often underestimated. At present a large number of monochromator designs have been developed, and we feel that it is now an opportune time to compare their efficacy for XAFS work. To accomplish this we are exploring the possibilities of organizing a workshop on XAFS monochromators, perhaps in conjunction with the next Synchrotron Radiation Instrumentation conference. We also plan to begin development of a test suite of monochromator characterization tests which could be used to compare the performance of different monochromator designs.

Finally we emphasize the importance of beam stability in determining the quality of XAFS experiments. This topic received significant attention in the previous report, but we continue to feel that many experiments are limited by the stability of the available beam. This is likely to be even more serious at the high brightness sources currently being built.

View of the Future

X-ray absorption spectroscopy should be recognized as growing in potential power and applications. The group wishes to emphasize that there is still ample room for instrumentation developments in the areas of sources, monochromators, and detectors. Concerning the new high brightness sources under construction, we would like to correct two widespread misconceptions:

1) There is some gain to be expected on photon statistics, but this is not going to be a real advantage unless considerable efforts are made to improve the *whole* spectrometer (stability, high quality optics, rejection of glitches etc.)
2) X-ray spectroscopy, just like scattering techniques can benefit from the use of new types of undulator sources featuring very high brightness. Typical examples include SEXAFS, linear/circular dichroism, time resolved experiments, and combinations of absorption and imaging techniques.

Unfortunately, improving the quality of the experimental apparatus does not necessarily mean simplifying the use of the instrument by external users. Therefore, for such sophisticated experiments more technical support will likely be necessary. This emphasizes the importance of careful consideration of the general users support questions raised previously.

REPORT ON LABORATORY XAFS

Group Leaders: Yasuo Udagawa and Samar Hasnain
Participants: Lidun Ma, Alain Fontaine, Kunquan Lu and several other workshop delegates

1. GENERAL

XAFS measurements at laboratories by the use of conventional x-ray sources can provide XAFS spectra of acceptable quality for structural study provided that proper precautions are taken. In laboratory XAFS measurements it is either photon statistics or systematic errors which limit the quality of the data. It is thus essential to eliminate systematic errors and maximize the available photons at the same time.

The major source of the systematic errors arises from the contamination of the white x-ray radiation from conventional sources by many strong characteristic lines from target material as well as its impurities, including tungsten evaporated from the filament. Even when I_0 is recorder, large intensity fluctuations due to these emission lines distort the XAFS spectra because of the finite dynamic range of detectors. Contamination of harmonics is another source of systematic errors which increases when the accelerating voltage is increased. Therer is also a trade-off between intensity and resolution .

In a laboratory XAFS setup an individual experimentalist can optimize experimental parameters (target material, monochromator crystal, detector, source operating voltage) to suit a particular experiment. The following are issues which need to be considered in a laboratory XAFS measurement.

A. Weak X-ray Intensity

. use of rotating anode x-ray generator and/or focusing geometry with bent crystal monochromator.
. dispersive geometry with one dimensional detector.
. evacuate beam path or place a helium bag to reduce absorption and scatter.

B. Inhomogeneous Spectral Distribution

. elimination of tungsten from anode by regular cleaning.
. feedback system to smooth the intensity distribution of the source.
. detectors with large dynamic range

C. Contamination of Higher Harmonics

. suppression of higher energy x-rays by operating the source at lower voltage.
. by a correct choice of monochromator crystal plane.
. solid state or scnitelation detector.
. double crystal monochromator

D. Resolution for XANES or at High Energy Region

. use of high order reflection or high index crystal cut.

2. Data Collection Modes

There are several detection modes for laboratory XAFS measurements with their own advantages and disadvantages. In the following, recommendations and evaluations concerning each mode are presented in detail.

2.1 Direct transmission measurement by scanning mode

Direct transmission measurement using step-by-step scanning of monochromator is the most commonly employed mode on synchrotron radiation sources. A plane crystal monochromator may be used, but spectrometers with a bent crystal employing Rowland circle focusing

geometry can supply an order of magnitude more intensity [Y.Udagawa, The Rigaku Journal, 6, 20 (1989)]. In this system both bent (Johann) and curved and bent (Johannson) crystal have been employed. A Rowland radius of about 300 mm has been used as the best compromise between resolution and intensity.

Various index planes of LiF, Si, and Ge can be used in the monochromator. For the high energy region however, high indexed planes of Ge are the only choice because the penetration of hard x-rays into light elements decreases the resolution of LiF and Si.

It is recommended that I_0 and I_t are measured simultaneously by using a semi-transmitting ionisation chamber or a proportional counter for I_0 detection. If I_t and I_0 are measured alternatively by placing the specimen in and out of the beam, reproducibility of the sample position must be carefully checked. In this case, the data is subject to source fluctuations.

The use of a solid state detector to detect I_t is preferable in that evaluation and elimination of the effect of higher order harmonics or scattered x-rays is most efficiently carried out by monitoring its output. Other detectors such as a scintillation detector is perfectly adequate for monitoring harmonics. Selections of the proper monochromator crystal plane and source operating voltage are most effective in eliminating harmonics. Detectors must be operated within their dynamic range.

When a high order reflection from monochromator crystals is used to achieve high resolution, lower as well as higher order reflections are always contaminated. The reflection of the desired order can be picked out by the use of a combination of an SSD and single channel analyzer. Filters are helpful to reduce lower order reflections. A double crystal spectrometer is the best choice for this purpose especially in the high energy region (>15 keV).

Large intensity variations due to characteristic lines are a major source of distortion in XAFS spectra and can be reduced by a feedback system.

Energy calibration of the monochromator can easily be done with conventional x-ray sources by making use of the emission lines of the target material or tungsten. Energy resolution can be checked at the same time as FWHM of the emission lines. It must be noted, however, that natural widths may be comparable to or even broader than those of monochromator resolution [S.I.Salem and P.L.Lee, At. Data Nucl. Data Tables, 18, 233(1976)].

2.2 Fluorescence Detection

XAFS measurement by fluorescence detection is more effective than the direct transmission mode for very dilute systems (Hasnain et. al. J.Phys.E. 17,40 (1984)) in laboratory XAFS as well. It is also indispensable for specimens on x-ray opaque substrates.

To cope with weak signals, detectors should subtend as large a solid angle as possible; thus, a combination of several scintillation counters is appropriate. Elastic and Compton scattering photons are the major source of background, and filters composed of a Z-1 element must be employed to reduce them. Optimum thickness of the filter should be chosen by measuring the $F / \sqrt{(F+B)}$ for different foil thickness (Baines et. al., Nuclear Instr. & Methods, A246,565 (1986)).

2.3 Transmission measurement by dispersive mode

The dispersive mode using position sensitive detectors is superior in principle because the whole spectrum of interest is measured simultaneously.

This mode has been tried with various position sensitive detectors such as a photographic plate, a silicon diode array or a position sensitive proportional counter. None of these can discriminate higher order reflections of the monochromator crystal. The dynamic range of photographic plate is limited and it is recommended that a pack of film is used to extend the dynamic range. This is a commonly used technique in protein crystallography on synchrotron radiation sources, where photographic film still remains a popular mode of detection. Recent

development of image plate system (Amemiya, Chapter 12 in Synchrotron Radiation & Biophysics, ed. S. S. Hasnain 1989, Ellis Horwood, U.K.), which has a high dynamic range, looks very promising.

3. Checklist for Experimental Procedures

The following list of experimental conditions/parameters is recommended to record in the logbook and in papers:

3.1 X-ray source
target material, operating voltage, and current

3.2 Monochromator
. mode of measurement (transmission or fluorescence)
. Optical geometry (dispersive or scanning)
. measurement time
. monochromator crystal, reflection plane, and slit width(s)
. energy resolution and energy calibration (by which line)
. harmonic content or how it is eliminated

3.3 Detectors
type of the detector used (detail should be given with reference to count rate, dynamic range etc.)
type and thickness of the filters if used

3.4 Good Experimental Practices
. Precautions about sample preparation is the same as for experiments at SR facilities.
. Measure a blank with appropiate mx. This is essential if dispersive geometry is used and will enable to correct for the non-uniform I_0 spectrum.
. Collect several spectra to check reproducibility and average them to improve S/N.
. Increase data collection time with at least k^2 so as to account for the decreasing EXAFS amplitude with k.

Subgroup Report on XAFS Database

Group Leader: B. A. Bunker
Participants: Dale Sayers, Tim Elam

I. Overview
The International XAFS Database is proposed to allow access and monitoring of the quality of XAFS data, facilitate cross-checks between groups, provide corroboration of experimental results, and to minimize the duplication of effort. The database will facilitate exchange of data, software, and other information relevant to the international XAFS community:

- •reference spectra
- •published spectra
- •calculated scattering amplitudes, phases (k,r,q)
- •help libraries
- •software for analysis, data collection, and theory
- •bibliography and abstract database
- •bulletin board, teleconferencing

II. Detailed Contents of Database

•reference spectra

These entries are spectra of known chemical compounds, and are useful in data analysis, verification of analysis methods, and in teaching. They will be subjected to scrutiny before inclusion in the database. Multiple entries will be included.

•published spectra

Because of space limitations, it is not possible to publish all the data used in a publication. Access to this data is absolutely necessary to critically evaluate the work.

The goal here is that virtually all XAFS publications will have a corresponding entry in the database. In other fields, it is common for journals to require the authors to submit their data to a database. It is clearly appropriate in the XAFS community as well.

•calculated scattering amplitudes, phases (k,r,q)

These tabulated values are extremely useful in data analysis, and their widespread availability would greatly benefit the community. A particular advantage to on-line access is the the codes are continuously improving and the tables therefore also need updating.

•test suite of data for training

This database will include entries of data through various analysis steps. This provides a software verification suites as well as reassurance for those learning analysis techniques.

•help libraries

This section includes a number of machine-readable documents: help text for various software packages, tutorials on XAFS, proceedings of workshops, etc.

•software

- analysis
- data collection
- theory

•bibliographic, abstract database

It is hoped that resources will be sufficient to provide an on-line abstract database for publications related to XAFS.

•bulletin board, teleconferencing

This facility would provide a platform for discussions, presentation of recent results, announcements of meetings, etc.

II. Access

The database will be available internationally via:

1) Networks:
   Interactive:e.g. Internet, HEPNET
   E-Mail: e.g. Bitnet
2) Tape
3) Telephone
4) possibly CD ROM

Except for a possible media charge for tapes, no access fee is envisioned at this time. Users would contribute data using the same methods.

III. Review of Contributions

At least in early stages of the database, explicit refereeing of contributed spectra is not foreseen. However, the contributor will be required to include the following information:

•synchrotron source and experimental station
•beamline optics
•monochromator characteristics

(e.g. type and number of crystals, focussing, etc.)
•mirror characteristics
•detector characteristics
•sample preparation techniques, including an estimate of thickness, particle size, and any other relevant information
•sample temperature
•discussion of energy calibration: preferably quoting the measured edge energies of the edge of interest *and* another edge near the end of the scan. This is particularly important for many fixed-exit monochromator designs.
•estimate of energy resolution, including monochromator resolution and description of method used to make estimate
•estimate of harmonic contamination, including a description of method to reduce the effect of harmonics
•comments by the experimenter, and additional comments by possible referees or other contributors

IV. Proposal for Implementation: National Nuclear Data Center

The National Nuclear Data Center at Brookhaven National Laboratory has offered a database service to the nuclear physics community for approximately 30 years. Representatives from this organization have recently decided to expand their operations to include x-ray data such as scattering cross-sections. On hearing about the report from the last XAFS Standards and Criteria Workshop, they have approached the Database Committee about also including EXAFS data. The representatives from the NNDC propose offering a database service as described previously in this document. The advantages of joining forces with an existing facility are:

(1) There is an economy of scale. This approach is much less costly than purchasing computer equipment and staffing our own center.

(2) The staff at NNDC have experience running an on-line database, and have worked through the problems that inevitably arise running an operation such as this.

Obviously, the NNDC will require some additional resources to accomodate the EXAFS database. We are currently exploring options for this.

At this workshop, we have unanimously approved the motion to run a pilot project, with a local group contributing data and software, to test access (both domestic and international) and general usability of the NNDC environment.

Committee on Implementation, Education and Experimental Facilities

Group Leader: Diek Koningsberger
Participants: Tim Morrison, Tim Elam, Grant Bunker

There are a large number of Synchrotron radiation centres where XAFS is major activity. A committee is to be set up, after consultation with the IAC, in order to facilitate the implementation of workshops' recommendations.

Facility	Location
SSRL	Stanford/USA
NSLS	Brookhaven/USA
CHESS	Cornell/USA
APS	Argonne/USA
ALS	Berkeley/USA
SRC(Wisconsin)	Stoughton/USA
Photon Factory	Tsukuba/Japan
LURE	Saclay/France
ESRF	Grenoble/France
SRS	Daresbury/UK
HASYLAB	Hamburg/W-Germany
BESSY	Berlin/W-Germany
ADONE	Frascati/Italy
-	-/Taiwan
-	-/China
-	-/India

I. Implementation and Dissemination

a) Checklist of required information for EXAFS papers to be sent to journal editors

It is not yet clear to what extent the synchrotron sources should be held responsible for bad science (poor quality XAFS data and improper or insufficient data-analysis). It is, in our opinion, a shared responsibility together with the different synchrotron user's institutions. We are concerned about the current reputation of XAFS research, in many communities. To improve this we must agree upon a list of minimum requirements for EXAFS papers and disseminate this list among the users and the editorial boards of the major refereed journals which publish XAS papers.

Proposed Actions:

•Neville Greaves and Diek Koningsberger will draft a letter.
•Grant Bunker will distribute the draft to all members of the workshop and contact persons of the different synchrotrons.
•York organization will disseminate the draft at XAFS VI.
•Journal editors will be contacted for comments on the proposal. Some examples:
  •Tim Morrison: Phys. Rev. Lett.
  •Neville Greaves: Nature and J.Non. Crystalline solids
  •Britt Hedman: JACS and J.Inorganic Chemistry

b) Creation of mailing list of X-ray absorption users

Attempt to create new comprehensive mailing list. Draw on mailing lists of synchrotron facilities and list of registrants for the York meeting.

c) Synchrotron Radiation News

Use Synchrotron Radiation News to communicate with users; give them the new users list.

d) Publish results of the Brookhaven workshop in conference proceedings York meeting

e) Establish a prize for best paper or new instrumental development in the field of X-ray Absorption Spectroscopy

Much like the various awards of the American Chemical.Society, it may improve visibility of high quality work and thereby encourage scientists to produce optimal quality science.

II. Education and Training

a) Training inexperienced users (local)

Synchrotron radiation is a valuable resource, and we believe that one of the tasks of the various synchrotron radiation sources is to set up training sessions for learning data collection procedures and analyzing XAFS data. This is may be also a combined task of the user community and the people responsible for running the XAFS beamlines (e.g. PRTs). It is the intention of Tim Elam, Tim Morrison, and Grant Bunker to publish an EXAFS cook book, which can be used to set up an x-ray absorption experiment and to optimize an EXAFS station.

It is also proposed to create a workshop group to help provide materials and support to local organizations interested in running a training workshop. In this way it is hoped to not only stimulate more workshops but also to assure that complete and standardized material is made available.

b) Advanced level (international)

Activities may include:

1) organization of summer/winter schools for theory and data-analysis at an advanced level.

2) workshops for special instrumentation, e.g. evaluation of monochromators for X-ray absorption experiments.

III. Cataloging Facilities

a) List of existing facilities for X-ray absorption experiments

Britt Hedman is making an comprehensive list of experimental stations for X-ray absorption experiments at all existing synchrotron facilities.

b) Recommended minimum beamline equipment.

1. Station set-up

- Detectors (ionization chambers, fluorescence counters etc).
- Electronics (e.g. amplifiers, V/F converters).
- Motorized slits
- Documentation must be available describing:

  a) calibration of X-ray monochromator
  b) characteristics of the monochromator (and mirror(s) if present)
  c) characteristics of the electronics
  d) schematic diagram of interconnections between electronic components.

It is not the task of the station master to optimize the station for each individual experiment, but enough information must be available that an individual user can do this him- or herself. The differences in background and orientation between chemists, biologists and physicists must be kept in mind. Ultimately it is the responsibility of the user to take the time to learn how to optimize an experimental station.

2. Equipment for user experiments

- motorized sample stage
- standard sample holders for liquids
- standard sample holders for powders
- sample press with dies suitable for a particular beam size
- dewars for standard powder and liquid sample holders capable of liquid nitrogen temperatures
- fluorescence detectors

3. Beam performance

- Monitor for beam energy and current
- Monitor for beam position and intensity

We have to make a strong case for the last monitor, because we have now enough evidence that beam stability is crucial for collecting good data. At some facilities the beam must be kept stable to better than 20 μ. This is important also in relation to the planned 6 GeV sources. Evaluating the detailed noise measurements, which have been performed in Daresbury, shows that photon statistics is not as important as low frequency beam noise in determining the overall performance of the XAFS stations.

c) Standard performance test of XAFS beamlines

1. Status of a particular beamline to be checked regularly by station masters/and or users

A very simple test experiment can be carried out for XAFS beamlines for energies above 3 KeV. The overall performance of the station in combination with the behavior of the x-ray beam should be checked at different energies. Aluminium foils with a total thickness giving an absorption in transmission of $\mu x=1$ can be measured at a particular energy with normal scan parameters under normal experimental conditions. The background can easily be removed and the noise pattern and amplitude can be measured and compared with previous test data collected under identical conditions. Phantom EXAFS oscillations, glitches, low and high frequency noise can easily be determined.

2. Quality determination of XAFS stations and international competition

It will be proposed to set up an international test for XAFS beamlines. The simplest test experiments to be carried out to get an impression of the performance of each individual XAFS station is to measure well defined Aluminium foils in transmission mode. Each test will be performed under identical scan conditions at several energies:

V K-edge :	5450 eV	Cu K-edge:	8990 eV
Pt-L_{III} edge:	11564 eV	Rh K-edge:	23219 eV

The results must be analyzed by an independent institution. The results will be published by Synchrotron Radiation News.