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ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

ANL/APS/CP-5

PROCEEDINGS OF THE FIFTH USERS MEETING FOR THE ADVANCED PHOTON SOURCE

Held at Argonne National Laboratory
October 14-15, 1992

December 1992

work sponsored by
U.S. DEPARTMENT OF ENERGY
Office of Energy Research

FOREWORD

Despite a downpour minutes before it began, the tour of the Advanced Photon Source (APS) facility was the undisputed highlight of the Fifth Users Meeting for the APS, held on October 14-15, 1992. More than 320 prospective users attended the two-day conference at Argonne National Laboratory (ANL), which was sponsored by the Advanced Photon Source, the ANL Division of Educational Programs, and The University of Chicago Board of Governors for Argonne National Laboratory.

The participants came to hear about construction and R&D progress, talk with representatives of major funding agencies, visit vendor displays, listen to scientific presentations, and, above all, walk the APS site to gain a sense of perspective and share the excitement of APS staff members at a point midway in APS construction. At the APSUO business meeting, six new members were elected to the APSUO Steering Committee. The current membership of the Steering Committee is shown below:

APSUO Steering Committee

Stephen Durbin, *Chairman* (Purdue)
Roy Clarke, *Vice Chairman* (Univ. of Michigan)

Haydn Chen (Univ. of Illinois)
Philip Coppens (SUNY/Buffalo)
John Faber, Jr. (Amoco Res. Center)
Doon Gibbs (NSLS)
Alan Goldman (Iowa State Univ./Ames Lab.)
Gene Ice (ORNL)
Samuel Krinsky (NSLS)
William Orme-Johnson (MIT)
Paul Sigler (Yale Univ.)
William Thomlinson (NSLS)
Keith Watenpaugh (Upjohn)

Bob Batterman, *ex officio* (CHESS)
Arthur Bienenstock, *ex officio* (SSRL)
Brian Kincaid, *ex officio* (ALS)
Denis McWhan, *ex officio* (NSLS)
Paul Horn, Past Chairman, *ex officio* (IBM)

Program Committee for the Fifth Users Meeting

Steve Durbin (Chair)
Bob Batterman
Alan Goldman
Keith Watenpaugh

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Proceedings of the Fifth Users Meeting for the Advanced Photon Source

ABSTRACT

The Fifth Users Meeting for the Advanced Photon Source (APS) was held on October 14-15, 1992, at Argonne National Laboratory. Scientists and engineers from universities, industry, and national laboratories came to review the status of the facility and to look ahead to the types of forefront science that will be possible when the APS is completed. The presentations at the meeting included an overview of the project, funding opportunities, advances in synchrotron radiation applications, and technical developments at the APS. In addition, the 15 Collaborative Access Teams that have been approved to date participated in a poster session, and several vendors displayed their wares. The actions taken at the 1992 Business Meeting of the Advanced Photon Source Users Organization are also documented.

WELCOMING REMARKS

Dr. Alan Schriesheim
Director, Argonne National Laboratory

Ladies and gentlemen, it is a pleasure to welcome you to Argonne National Laboratory to participate in the Fifth Users Meeting for the Advanced Photon Source.

Increased activity at the construction site brings us closer to the time when Collaborative Access Teams will come in to construct their beamlines. The abundance of paperwork that I have signed has moved through the system. The result is efficient and effective construction done on budget and basically on time.

I know that the future is getting closer because we are having frequent discussions about funding for the beamlines and where we're going to get money for beamline research programs. The continuing dialogue with the funding agencies is a sign of continuing progress of the Advanced Photon Source Project.

Periodically, Dave Moncton and I meet to discuss APS technical subjects, but the bulk of my job is to see that this project gets the proper attention from Washington. My perception is that no one in Washington has weakened, either in the agency or in the halls of Congress, in their support of the Advanced Photon Source.

In fact, if anything there is a stronger commitment. That has to be balanced with the obvious fact that money is not exactly plentiful. It doesn't rain down on our shoulders here at the Lab, and it doesn't rain down on anyone else's shoulders in the technical community. That is not surprising. We live in a very contentious system.

My commitment to you is to continue to use whatever clout the Director's office has to bring this endeaver to fruition . It is the highest priority project within the laboratory. It continues to get the attention that a project with that priority deserves.

So welcome again. I look forward to seeing you tonight.

Status Report on the Advanced Photon Source - Fall 1992

by

David E. Moncton
Associate Laboratory Director for the Advanced Photon Source
Argonne National Laboratory, 9700 S. Cass Ave., Argonne, IL U.S.A.

1. Opening Remarks

Welcome to the Fifth Annual Advanced Photon Source Users Meeting. We seem to hold one of these annual meetings every 18 months. We cannot help but keep the project on schedule given that definition of a year. There has been substantial progress in every area of the project. I hope the next day or two will give you a clear picture of that progress.

2. Staffing

Project staffing is nearly complete with the exception of some additional technical people for installation work, and perhaps another 25% added to the staff of the Experimental Facilities Division (XFD). Total staff currently numbers approximately 400. We have made some key appointments at all levels during the past year or so. We hope you are able to come into contact with some of our staff during this meeting, and that you get a feeling for what we believe is an excellent organization. We are particularly pleased to have had Edward Temple here for the last year and a half as Project Director. Yang Cho, who was Project Director at the outset, did an excellent job in that capacity. He was a critical factor in bringing the project to its early successes and now he is concentrating his efforts on development of plans for commissioning and operating the facility. He also has other, part-time interests in the possible development of a spallation neutron source at Argonne.

3. Schedule and Cost

As in the past, we want to be honest with the user community on the subject of schedule, so that you can take all of our plans into account as you develop your plans for beamlines. As we look at the project today we see some pluses and some minuses. On balance we would say that the project is a quarter of a year behind the baseline schedule that we had set up some time ago. We do not think this is an obstacle to meeting our future milestones, and we have developed a number of plans to accelerate activities and thereby regain ground on our schedule. Whether or not we are able to carry out these plans depends to a large degree on the funding situation for FY93.

As of the end of FY92, the Project has committed $205M, or essentially half the purchasing power of our construction budget. As far as the budget estimates for where we are to date and what we believe it will cost to finish this project, we have over the last year used a significant portion of our contingency fund. Nevertheless, we feel comfortable with the amount of contingency that remains. It is still 15 percent of our cost to complete. We strongly believe that this project will come in at a final cost that is within the original cost estimate.

The issue that we are most concerned with at the moment is our FY93 funding level. We have received word that the Department of Energy (DOE) wishes us to reduce our FY93 expenditures. Fiscal year 1993 had been scheduled to be our peak construction year. The funding for FY93 was planned to be $110M. We have been directed to begin the new fiscal year with expectations of receiving $14M less than that level, or $96M. We are now working to develop a detailed plan for proceeding with our work under the new funding limitations, and to assess the potential impact of that reduction. There is a chance that we might see some restoration of those dollars at some time during the course of the fiscal year.

4. Reliability

We had a very exciting workshop here last January on the subject of accelerator reliability. People from various accelerator installations, including the Superconducting Super Collider, the Continuous Electron Beam Accelerator Facility, and the Cornell High Energy Synchrotron Source, met to discuss accelerators in terms of what causes them to be unreliable and what can be done to raise the level of reliability. That workshop has led to a number of follow-on studies. Experts from the engineering schools in the local academic community have been working with us on particular problems, trying to use some of the more systematic techniques of reliability engineering to help us improve the reliability of various accelerator subsystems. We are very pleased with that effort. In addition, we are anxious to work with existing facilities, which have a wealth of operational data that can be very useful in characterizing reliability problems, and gain an understanding of what really is in store for us, while at the same time helping the existing facilities to better understand their problems.

5. Facility Construction

The status of conventional-facilities construction as of two weeks ago is shown in the aerial photograph of the APS site (Fig. 1). The entire complex is well along. The Project is looking forward to the challenge of moving into the installation phase, and then seeing the first accelerated beam.

The Experiment Hall is in various stages of completion. Concrete has been poured for about 3/4 of the Experiment Hall circumference. We are now awaiting completion of the vehicle underpass, which will provide access to the infield. Once that underpass is complete, we can abandon the temporary access road currently in use. We will then finish the concrete work in the southern portion of the Experiment Hall. In the next few weeks, we hope to complete all of the concrete work for the Experiment Hall and the Storage Ring Tunnel. Experiment Hall steel has been erected around more than half of its circumference.

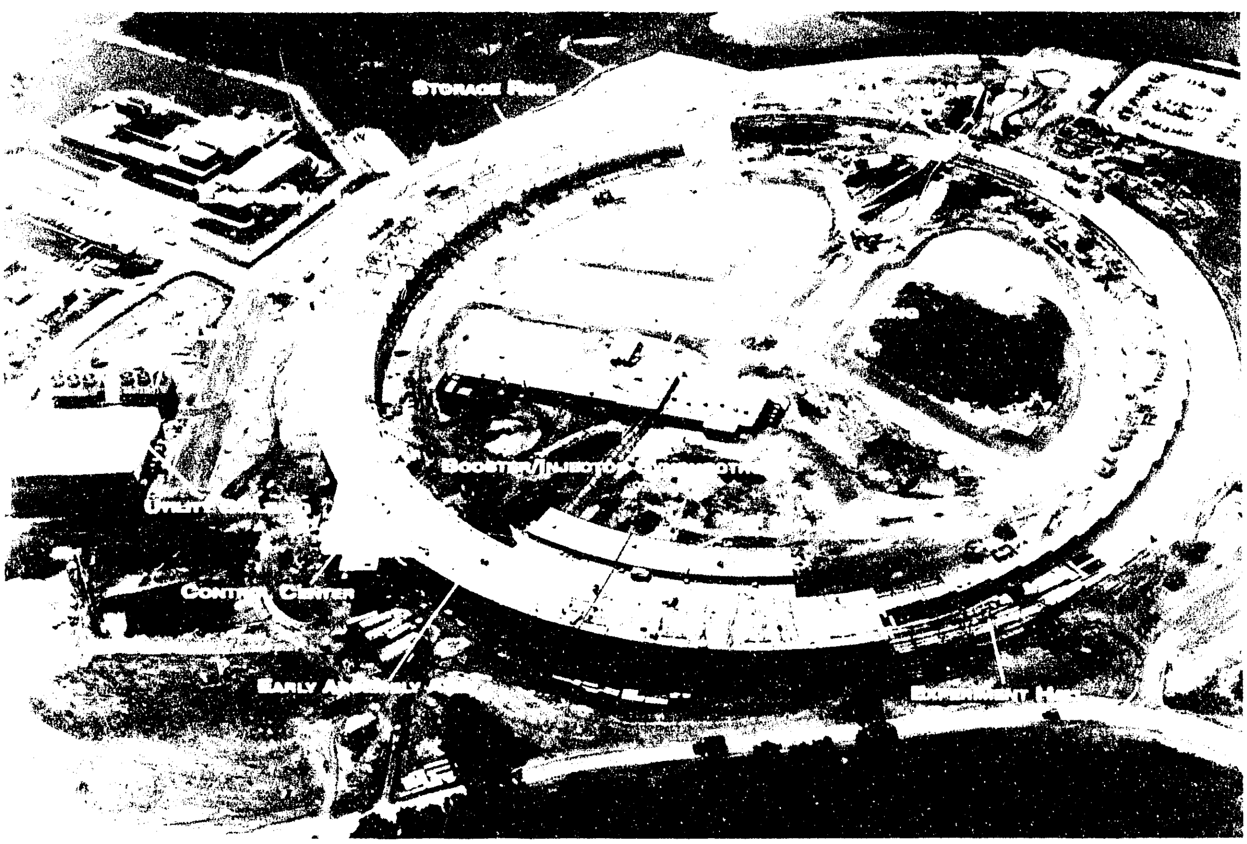


Fig. 1. The APS facility as of September 29, 1992.

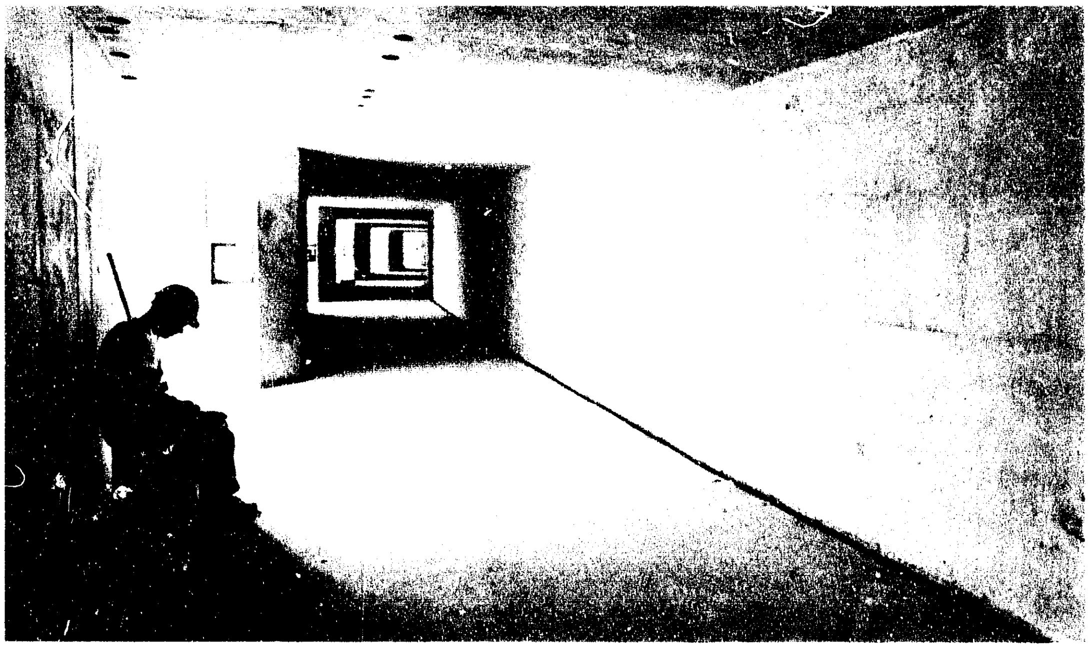


Fig 2. The interior of the Storage Ring Tunnel.

The first portion of the Experiment Hall to be occupied will be the Early Assembly Area (EAA). This is a region of the Experiment Hall devoid of beamlines and ratchet walls because of four straight sections that contain the three rf cavities and one sector that is used for injection. The EAA will serve as a staging point for the accelerator components from our production areas. These components include magnets, vacuum systems, and the girders upon which they will be mounted. The final assembly of those components will be done in the EAA just prior to installation in the respective tunnels. We need this building very soon in order to stay on our installation schedule. We anticipate occupancy in the next few months.

The Storage Ring Tunnel itself now exists around approximately 70 percent of the ring circumference. Figure 2 shows the interior of the Storage Ring Tunnel, with a lonely user waiting for beam.

The DOE has granted the Project beneficial occupancy of the linac and injection wings in the last few months. The Linac Group of the Accelerator Systems Division (ASD) is busy installing components in the linac tunnel. Figure 3 shows the first set of linac Helmholtz coils on the mounting girder in the electron-gun end of the linac tunnel. On the other side of the linac tunnel shield wall is the klystron gallery, where all the linac power supplies and support systems reside. Figure 4 shows the first modulator power supply and water control systems in place. The low-energy transport region of the synchrotron tunnel, where the linac intersects the synchrotron/ booster, is essentially complete (Fig. 5). Concrete work for the synchrotron tunnel is complete and the enclosure has been covered with earth. Utility work is ongoing inside the tunnel (Fig. 6), which is scheduled for occupancy in the very near future.

6. Accelerator Systems

The Accelerator Systems Division, under John Galayda's leadership, is staffed up to approximately 240 people. It is a truly excellent group. They have developed a set of impressive manufacturing capabilities out in the Argonne 300 area, some of which you will see in the course of this meeting.

6.1. Vacuum System

The Vacuum Facility is up and running. There are 40 sectors in the storage ring, each with 6 vacuum chamber sections, for a total of 240 chambers, including the straight sections for the insertion devices, which have a somewhat different cross section. Approximately 60% of the storage ring vacuum chamber extrusions have been delivered (Fig. 7). The first chambers have been machined to accept magnet pole faces and the various fittings that go on the chambers. Two computer-numeric-controlled welding systems (Fig. 8) are operational in the Vacuum Facility. These devices will perform a total of 2400 precision welds while attaching photon-absorber flanges and bellows connections to the chambers. We have invested a great deal of time over the last four years in an R&D program to make absolutely certain that those welds meet all specifications, and we are very pleased with the success of that program.

6.2. RF System

Radio frequency (rf) systems are difficult to make reliable, and they are critical to the performance of a storage ring. The ASD RF Group has spent a great deal of time on R&D to develop rf cavities that meet our specifications. Figure 9 shows the rf-cavity test stand, with a 1-megawatt klystron and the waveguides that feed power to the stand. This stand affords us the capability to test both synchrotron and storage ring cavities. We currently have on hand a prototype copper storage ring cavity (Fig. 10) and all four production cavities for the booster (Fig. 11). Full-power tests of these cavities have been very successful. We have just recently gotten very good news on a single fixed-price contract for procurement of all the storage ring

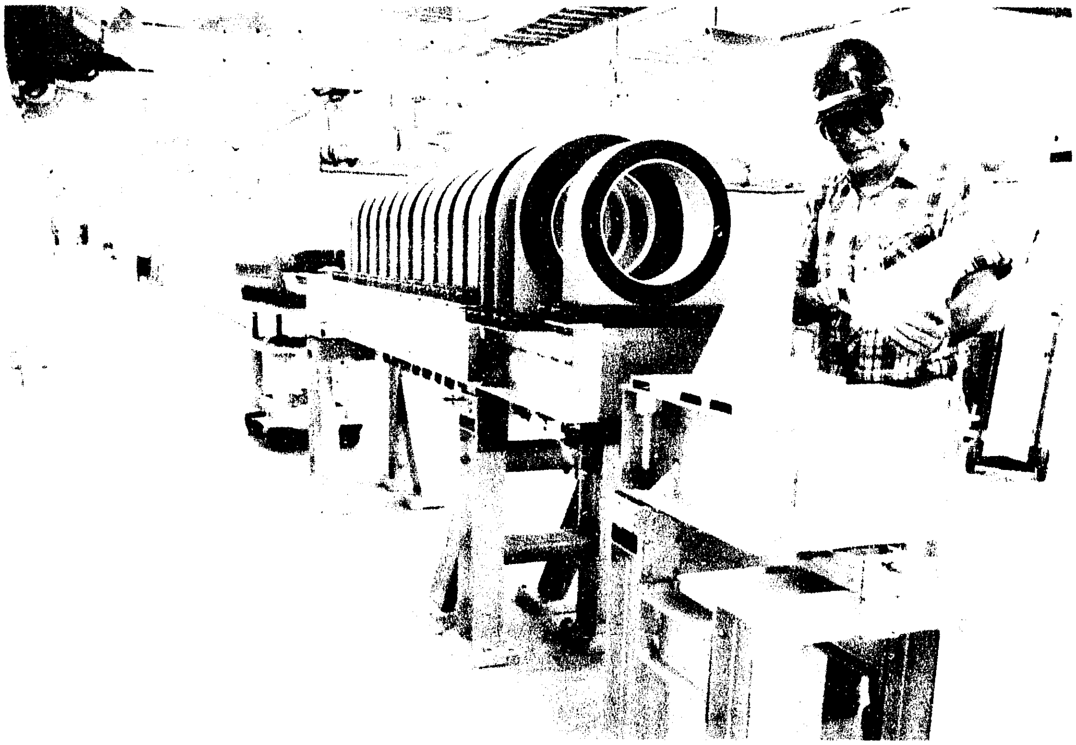


Fig. 3. Beginning linac installation.

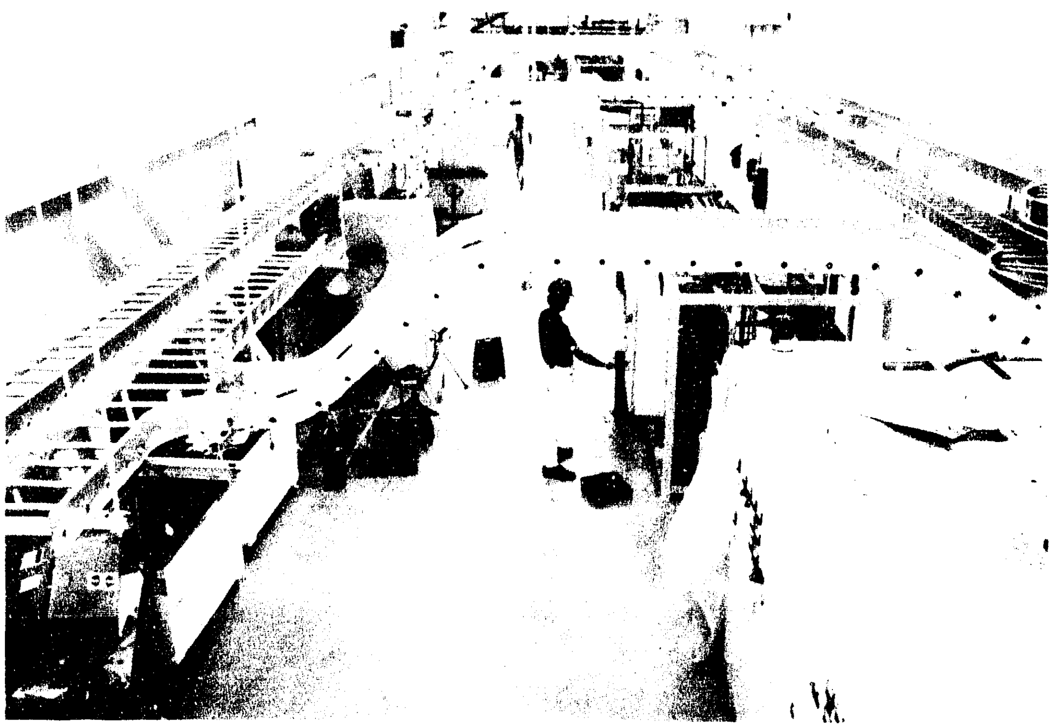


Fig. 4. The klystron gallery.

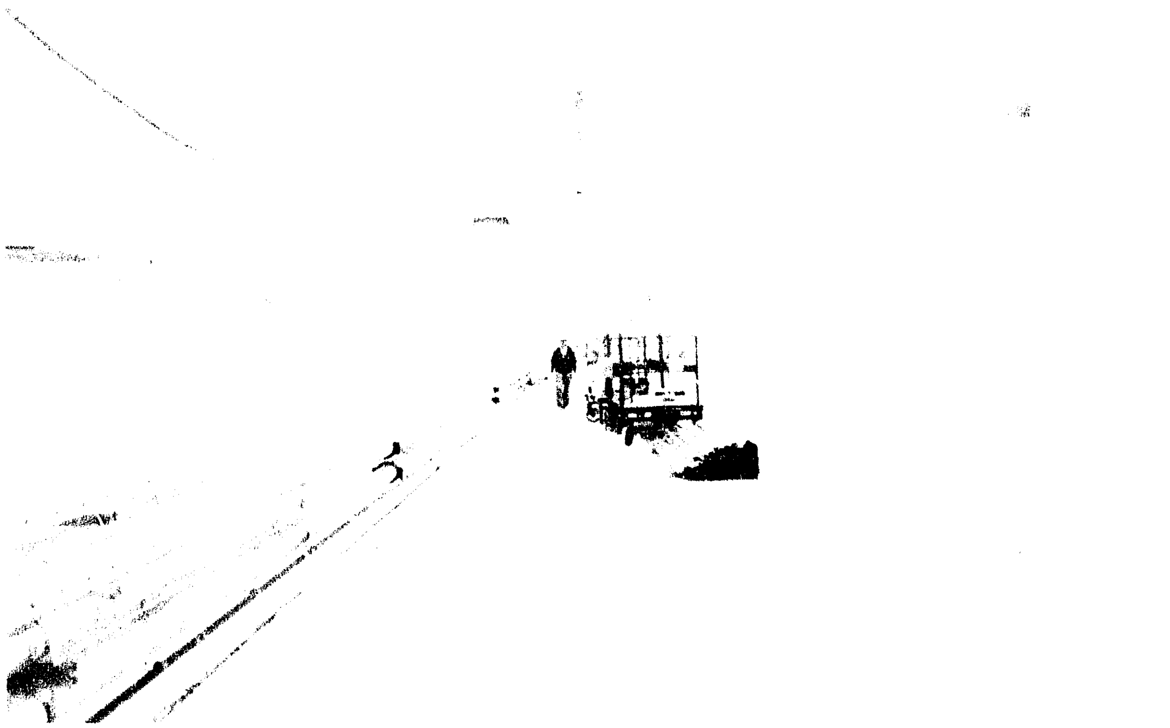


Fig. 5. The low-energy transport tunnel.

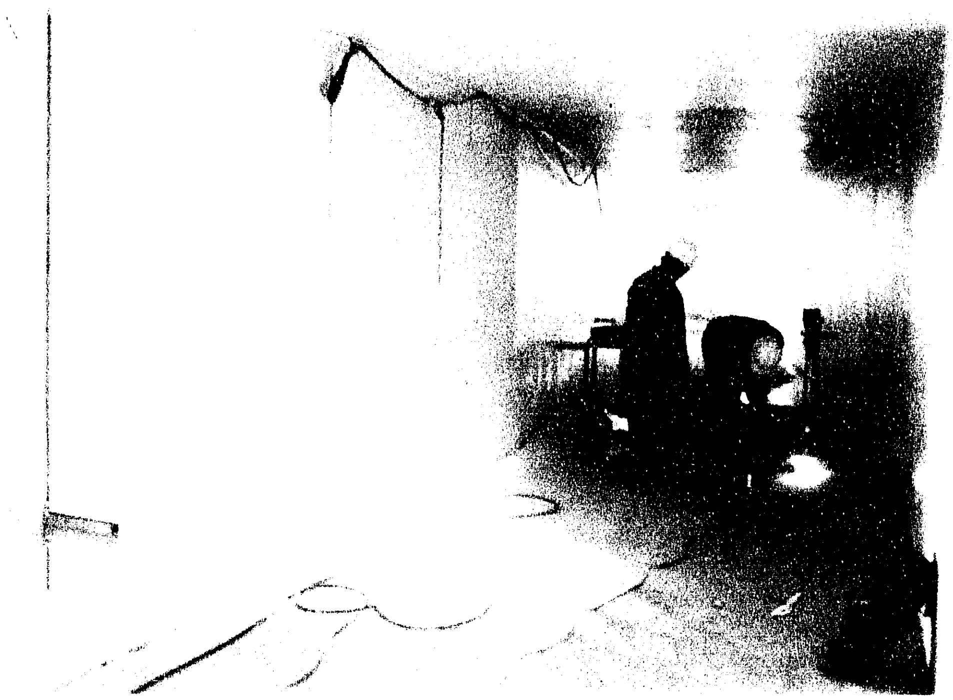


Fig. 6. The Synchrotron Tunnel.

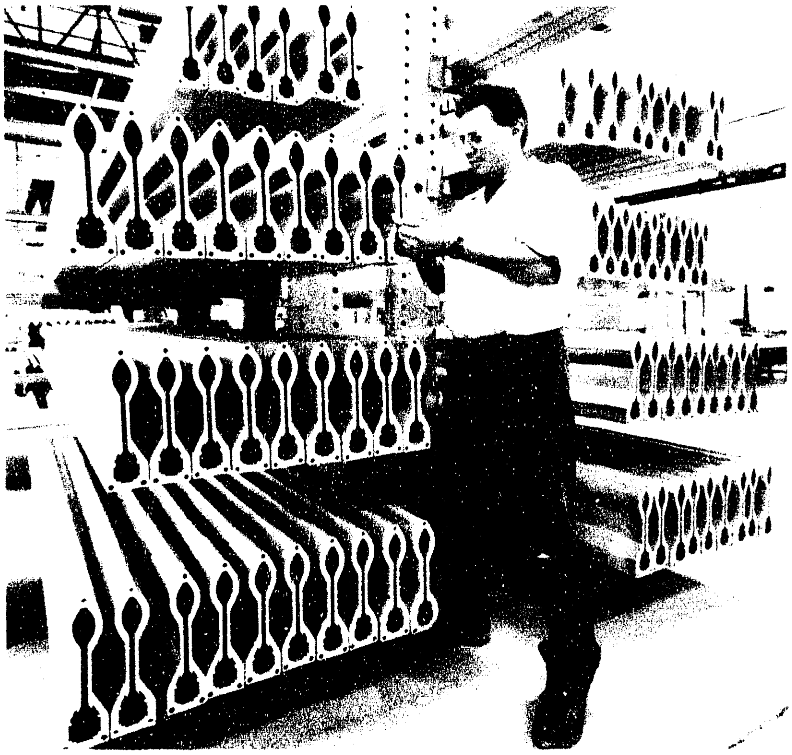


Fig. 7. Extruded-aluminum storage ring vacuum chambers.

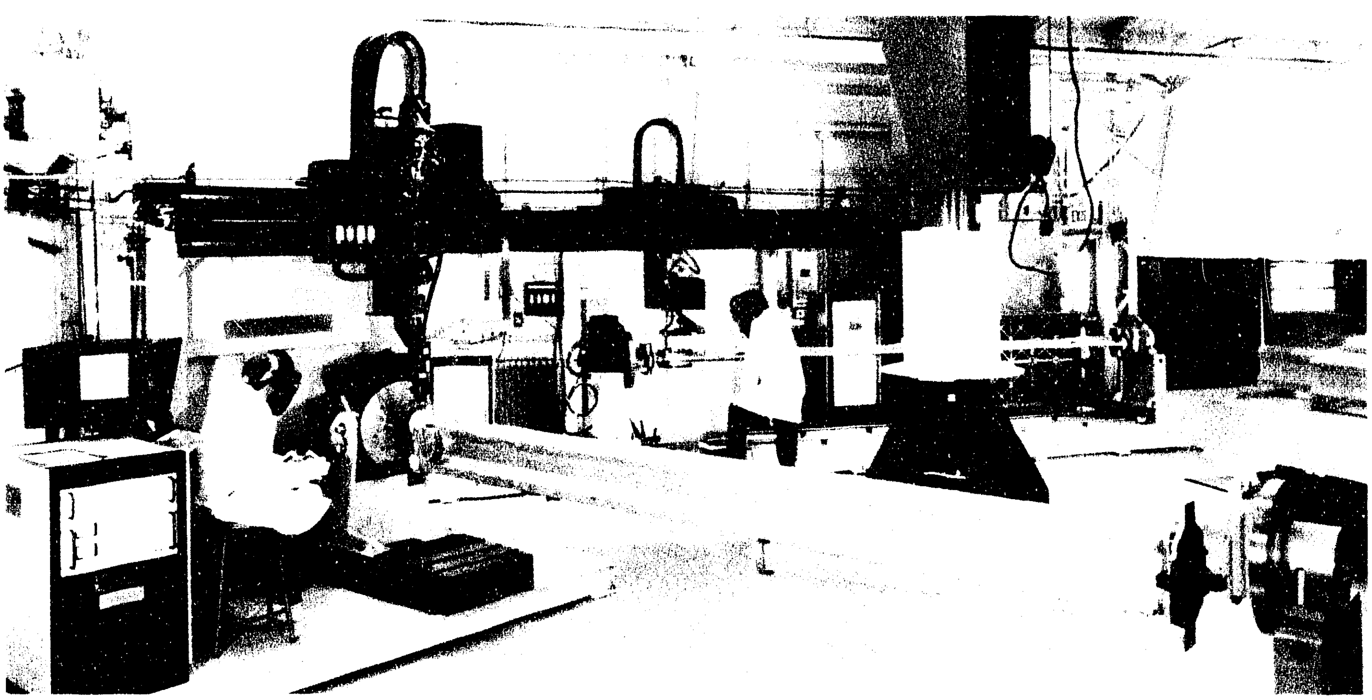


Fig. 8. Acuweld CNC-controlled chamber welding stations.

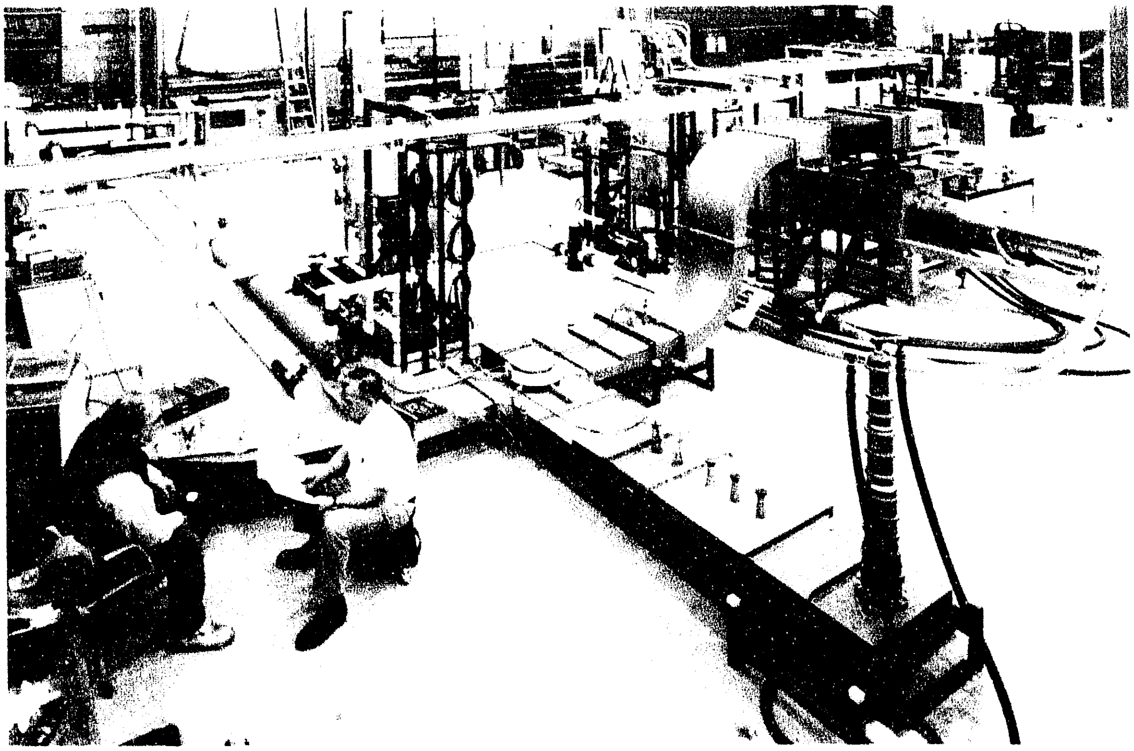


Fig. 9. The rf test stand in ANL Bldg. 371.

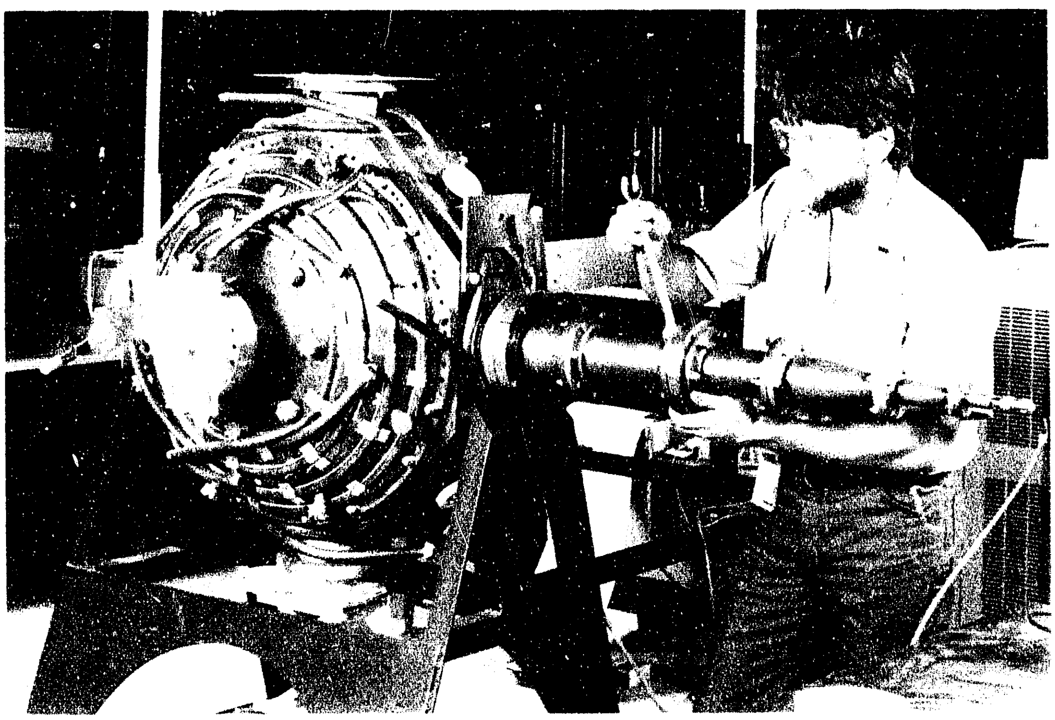


Fig. 10. Prototype copper storage ring rf cavity under test.

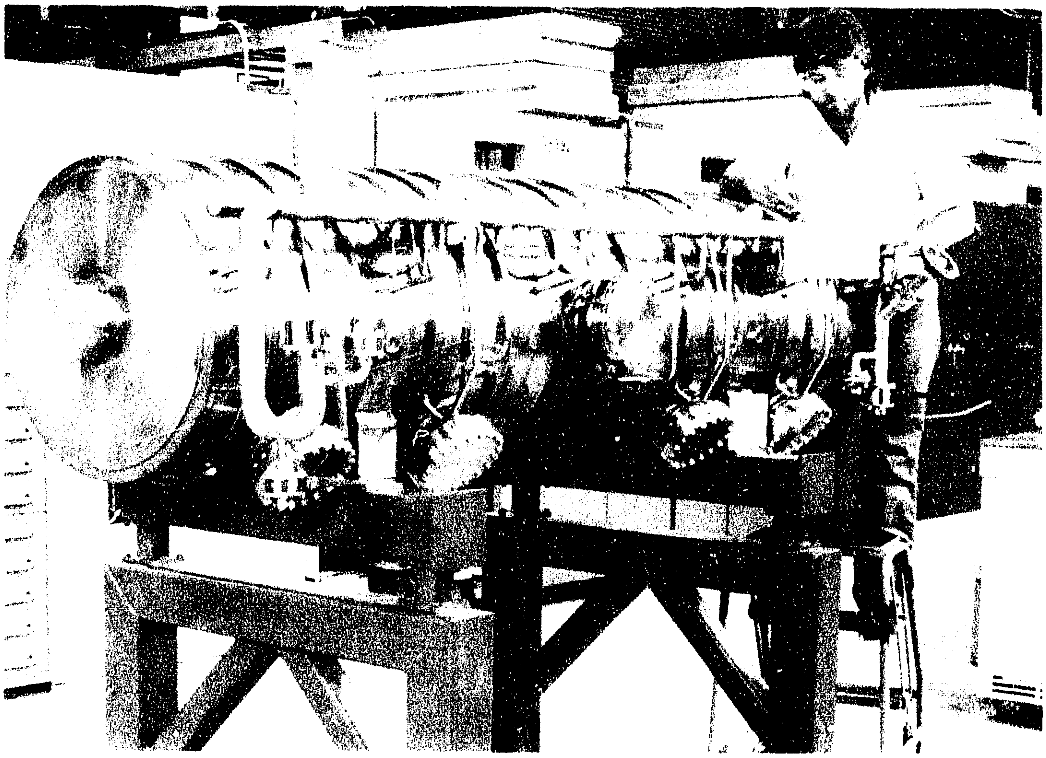


Fig. 11. Production synchrotron/booster rf cavity.

Fig. 12. Production synchrotron dipole bending magnets.

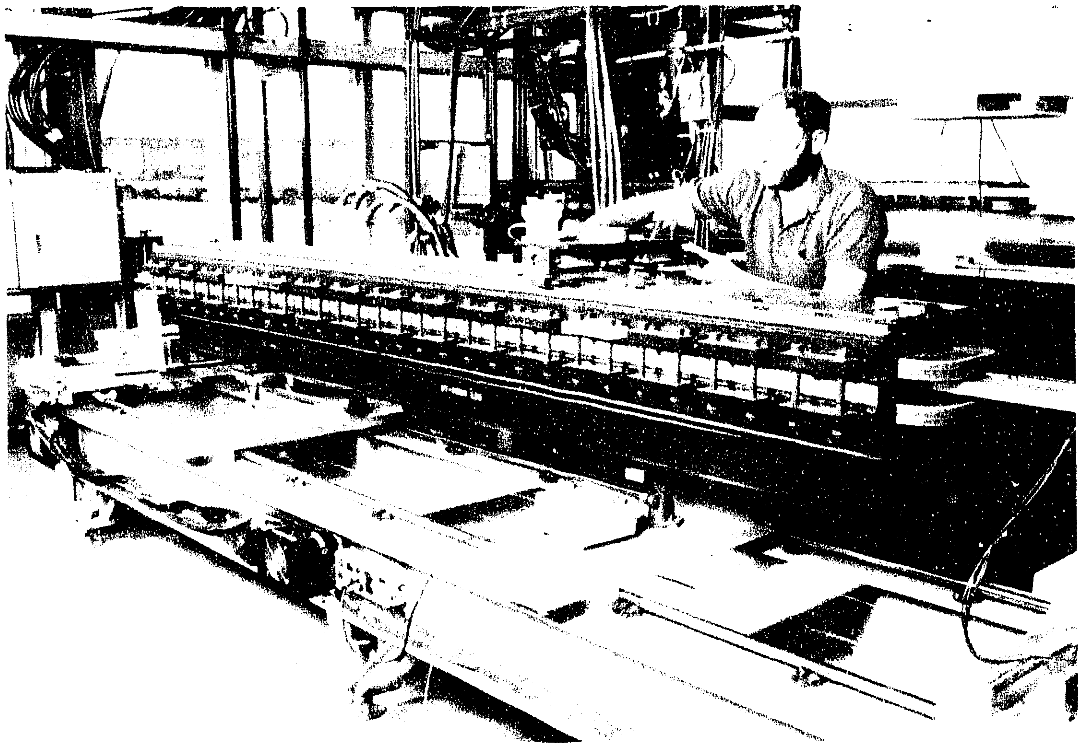


Fig. 13. Synchrotron dipole magnet on test stand.

cavities, including a number of spares. The costs in this contract are significantly under our baseline budget. We are also planning on having enough rf power in the storage ring to provide complete redundancy in anticipation of possible failure. That is, we will have twice the number of cavities needed to meet our minimum goal of 100 mA at 7 GeV. We have all spent too many hours at synchrotron facilities looking at screens that read-out "rf trip," or what have you, as the reason for loss of beam.

6.3. Magnet System

Producing accelerator-magnet prototypes proved to be a very useful exercise because we were able to discover problems in our magnet designs well before they cropped up in production units. We altered those designs as needed. For instance, we eliminated saturation in the quadrupole magnets. We changed the design of our storage ring sextupoles to remove a combined function of steering and sextupole focusing and separate those into two different magnets. Meanwhile, production has begun on a number of the magnets. Figure 12 shows several production synchrotron dipole magnets, with more being fabricated every week, both at Argonne and by industry. All of these magnets undergo rigorous testing. Figure 13 shows a synchrotron dipole on a test stand in our Magnet Measurement Facility. We are on the verge of beginning production on storage ring sextupole and storage ring quadrupole magnets.

6.4. Power Supply System

There is a whole host of other accelerator-related activities too numerous to mention in detail here. For example, the Power Supplies Group is involved in a rigorous program of procurement and in-house tests. Special temperature-controlled rooms are used to heat the power supplies up to high temperatures in the interest of gaining a better understanding of what their operational reliability will be. We will also conduct high-power tests in order to weed out the weak power supplies before they are installed. There is a frighteningly large number of power supplies in a machine like the APS, all of which must work in order to keep the beam circulating. When one multiplies the mean time to failure for every chip by the number of chips by the number of power supplies, one gets a mean-time-to-failure for the entire system of approximately 1 week. That is a daunting number. We are improving the designs of the power supplies by minimizing the number of components and by using components with high reliability figures. Those efforts have been somewhat successful. If we are going to achieve good power supply reliability, we will have to do a good job of diagnosing failures before they occur, making spares available, and making it easy to automatically determine which power supply failed in order to change it.

7. Experimental Facilities

The Experimental Facilities Division is close to all of your interests. This division, led by Gopal Shenoy, is ramping up rapidly in order to take on a very big job.

7.1. Insertion Devices

Undulators have been under design and test here for many years. We have constructed prototypes, and worked with both Cornell and Brookhaven to install prototype insertion devices and test their performance. We are satisfied with our understanding of all the performance parameters of these devices, particularly errors and how they deteriorate the synchrotron radiation that is produced. We feel very comfortable with the ability of the external vendor community to provide insertion devices that meet our specifications. We are ready to go out with the first package of procurements for the Undulator Type A devices, which will be the primary source of radiation for most beamlines. This procurement requires money, and we are concerned about our financial ability to place that order in FY93.

Research and development on undulators is going to be an ongoing activity for this project. There are a number of opportunities for enhancing the performance of insertion devices, and one

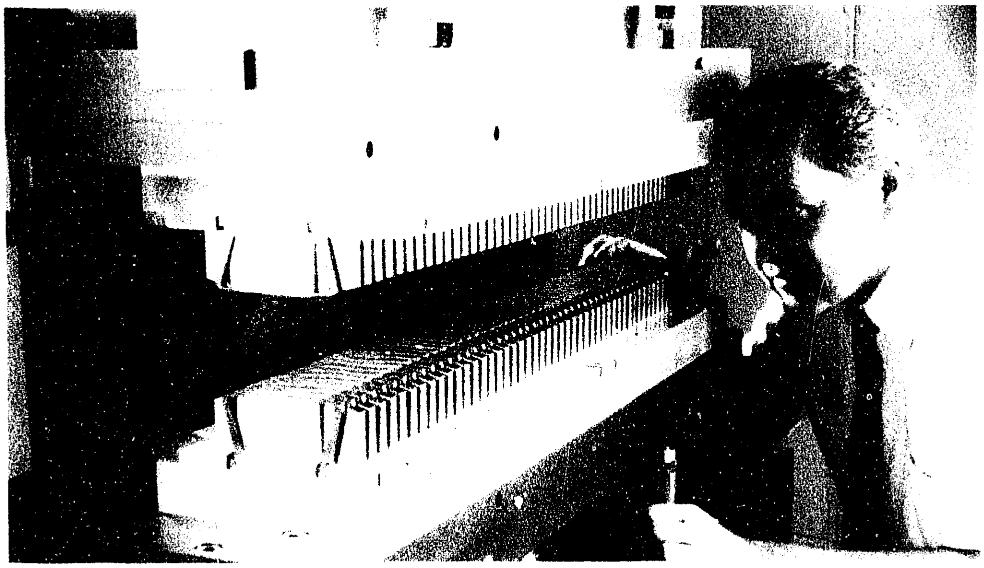


Fig. 14. Wedge-pole undulator from STI Optronics.

of those is the wedge-pole design (Fig. 14), which helps eliminate saturation regions in the poles and provides higher field at the same gap or permits use of larger gaps at the same field. In our case, we are particularly interested in pushing undulator technology to higher photon energies. I would like to see this machine someday produce up to 100 kV in the first harmonic. That will take some effort, but it is not out of the question. That development could have a tremendous impact on the range of science done at a facility like the APS.

7.2. Optics Cooling

High heat loads pose a major challenge for this facility and others like it because of the high brilliance and high power densities that are brought to bear. We must push the technology a number of orders of magnitude beyond what is necessary at bending magnets on current facilities. Several years ago, we started an R&D program to explore the use of liquid gallium as a coolant. This was a technology that had been part of the reactor program here at Argonne and was taken over and applied to the high-heat load problem with great success. We have recently spun off a small start-up company called Qmax, which is developing gallium-pump technology for cooling high-power electronics as well as rotating anodes used in commercial applications.

Hopefully, this company will be in a position to provide gallium pumps to be used in conjunction with our monochromators.

To further ameliorate the effects of high heat loads, we have developed a very innovative crystal geometry using a double crystal slanted at a very high angle to distribute the radiation over a much larger area. This geometry also has the secondary effect of orienting the crystal in such a way that the inevitable thermal bump, even though it is of a reduced magnitude because of the spread of the beam, is perpendicular to the diffraction plane rather than being in the diffraction plane. The result is that the diffraction profile is not distorted. The combination of optimizing the cooling channel geometry and this inclination of the crystals has produced a monochromator which has the inherent capability to withstand the power levels at the APS. It also has a broader scanning range than a traditional asymmetric crystal, thereby preserving the full tunability of this monochromator. The inclined geometry has been developed to the stage where a set of specifications have been written and we have received bids from two companies for producing the first prototype.

Another novel program is the use of chemical-vapor-deposition (CVD) diamond for two particular applications. One is as a blade for a photon monitor. Tests have shown CVD diamond to have properties considerably better than the metal blades which are currently used. This synthetic diamond is also being evaluated as a window material and perhaps even in a combined function device that would be both monitor and window.

The XFD Engineering & Construction Group has taken their designs for front-end components through conceptual design and Title 1 exercises, which is the first 30 percent of the work, and they are deep into the details of those devices. All users should be aware of the central design exchange, which is a computerized library of all the detailed designs that are being produced by both the APS staff and users. This arrangement allows all the parties involved to look at what is being done and exchange design information.

8. User Programs

8.1 Collaborative Access Teams

You are all aware of the extensive process that has taken place over the last three years in pursuit of research proposals. Beginning with Letters of Intent and then on through the formal proposal phase, to the review and acceptance of final proposals, all of the committees have worked very hard. These committees comprise members, drawn in the main from outside the APS, who have given generously of their time and energy to review proposals and make sure that the science done at this machine is of the highest order. That process has resulted in the approval of a very high-quality group of 15 Collaborative Access Teams (CAT), which, at this time, represent a wide-ranging group of more than 500 people from 80 universities, 26 industries, and 19 federal and private research laboratories. We are still open for business; anybody thinking about putting together a new CAT is more than welcome to submit a Letter of Intent, and if that is approved, to follow on with a formal proposal.

To date, five CATs have submitted conceptual design reports. The Instrument Feasibility Panel, under the chairmanship of George Brown, reviewed these CDRs a month ago, and will be meeting again in December 1992 to review a second set of CDRs. It is very exciting to see what everybody is planning to do. Some of us are a little bit overwhelmed with the job of putting all of this hardware on the Experiment Hall floor. But that is what we are here to do, and so we are very excited to see the actual plans emerging. We hope that the first Memorandums of Understanding (MOU) between Argonne and the CATs will be signed by early 1993. We have a draft MOU that is being reviewed by the users committee. We want to be sure that the MOU encompasses the needs of the APS as well as of the community, and that it is a document that can serve in the future as a basis for a very solid and business-like arrangement between the facility and the CATs. Management plans for the CATs are a prerequisite to an MOU signing. These plans are in the preparation stage, and will be reviewed upon submission.

Collaborative Access Teams have to up to now acquired some $50M in non-federal funding. Not all of this is money in the bank, but it is very heartening to see the success that the CATs have had so far in a very tough funding climate. Every CAT has not gotten every dollar that they wanted, but there are still a lot of battles being fought. Some of the funding agencies will need to look more carefully at their long-range plans and see how these activities are going to be incorporated. We at APS need to see statements of intent to fund beamlines from the various sources of financial support for individual CATs. We are prepared to make our funding commitments at the same time that the CATs make theirs.

8.2 Research Directorate

We have established a Research Directorate made up of myself and a number of our senior staff at APS, as well as the directors of each of the CATs. The Research Directorate meets on a quarterly basis, and those meetings have become very productive. We are learning how to develop a close working relationship.

8.3 Collaborative Research Program

The Collaborative Research Program is an opportunity for collaboration between APS staff and users with an interest in participating in the development of a particular instrumentation, but whose resources are not, in their judgment, adequate for the job they have to do. Our intent is not to act as a funding agency for the outside user, but rather to form teams comprising APS staff and outside users. These teams will focus on certain technical objectives that are judged by a panel composed of members of the APS staff, as well as members chosen from the users organization, to have an instrumentation objective that has some application or utility beyond an individual experiment. The process is working very well, as indicated by the number of instrumentation proposals that have been accepted by APS. Every year we put out a call for these proposals, so I encourage you to think about contacting us if you have some particular instrumentation idea in mind and you would like to team up with the APS to achieve your goal.

8.4 User Technical Interface Group

Gopal Shenoy has effected a very important organizational change by establishing a User Technical Interface Group whose function it is to act as liaison between APS and the CATs. This group is led is Steve Davey, and he has a big job to do.

8.5 User Housing Facility

In 1986, the State of Illinois pledged financial support for a user residence facility to be constructed on the APS site. We envision a 240-bed facility equipped with data links and various other amenities to minimize frustrations and make your stay at this facility as scientifically effective as possible. We would like to have this facility built in the FY94-96 time frame so that it is available early for users. The state's financial commitment was part of the package put forward by Illinois to convince the federal government to build the APS here at Argonne. That commitment was made by then-Governor James R. Thompson, and of course, we have a different governor in Illinois now. This state also has a substantial budget deficit now, as do many states. The result is that we are not exactly certain where this commitment currently stands. So we are going back into the system. We have done a design study for such a facility, we have chosen a site location, we have concept plans and a price tag. We are going to remind state government of its pledge of $15M to underwrite construction of the residence, which played a role in getting nearly 1 billion federal dollars into this state. That is, we think, a fairly good return on investment - $1B on a $15M investment.

9. APS Instrumentation Initiative

Because we are currently encountering difficulties in maintaining full funding for Phase 1 of our construction program, why talk about a Phase 2? We believe the APS will offer a tremendous research capability in terms of the kinds of science to be done here and the number of beamlines at which that science will be carried out.

As you all know, only about 60% of the 34 APS sectors, each with two beamlines, will be occupied during the first phase of research activity. We are drafting a proposal for DOE on a second construction phase, which we are calling the APS Instrumentation Initiative (APSII). The intent of APSII is to achieve full use of the APS by the year 2000. That proposal would call for the construction of the 4 (of a total of 8) laboratory/office modules not constructed under Phase 1. The proposal also posits the preparation of 8 additional sectors in the same style as the first 16, so that we would have a total of 24 sectors for Collaborative Access Teams using the same arrangements as we have for the first 16. That, of course, would leave 10 unfinished sectors. It is time for the community to think about the best way to use these additional facilities. The APS hopes to work with the users' organization in developing this concept by targeting opportunities for developing very specialized capabilities that may be outside the scope of what any individual CAT could possibly do. These capabilities would then be available to all the groups. We have developed a long list of candidate beamlines that fit in this category. We seek input from the users' organization collectively and from any of you individually. The intent is to implement 10 of these beamlines at the rate of 2 per year for a 5-year period.

As part of this program, we are requesting base funding for the front ends and insertion devices on these 10 beamlines, and also seed funding of perhaps $5M per year per. That level of support would minimize the amount of fund-raising that has to be done in conjunction with building the beamlines. We recognize that right now, the CATs are trying to raise money. We would like to get those commitments more up-front in APSII than they have been in Phase 1 and thereby avoid all of this cycling around. The cost of seeing this facility fully implemented on that time frame is on the order of $200M. We have submitted to DOE a Schedule 44 on this proposal with the idea that we could be ready to start as early as FY95. We will just have to see what the landscape looks like after the presidential election. We are likely to see substantial changes in the DOE as a result of the trickle-down effect of an election. We are looking forward to the opportunity to work with some new people at the top of the DOE and to work with the people that we consider our close friends in the program office who, hopefully, will still be there after the election.

Basic Energy Sciences Support for APS Beamlines

William T. Oosterhuis
Division of Materials Sciences/BES, ER-132
U.S. Department of Energy
Washington, DC 20585

I am happy to be here, and I would like to welcome you on behalf of the DOE.

Today, I would like to make a few remarks about funding for beamlines at APS, how to go about it, who to contact, and the prospects for success in getting the necessary support.

I know that we have a big job ahead of us - the funding situation is very difficult this year in FY93 for all federal funding agencies. It is clear that in order to get a reasonable complement of instrumentation of the experimental floor in time to make use of the first x-rays from APS, that it will require a coordinated effort by several federal agencies, as well as by universities and industry. We had hoped that the FY93 budget would be much better than it has turned out to be. Never-the-less, I believe that we are making progress in getting some efforts started even in this difficult year of FY93. You will hear from several of these federal agencies (NSF, NIH, DOE) as we go along today.

First of all, let me put forth a fundamental principal which I and my colleagues in the agencies have accepted: If I am willing to support a research effort, then I should be willing to provide the necessary instrumentation to carry out that research. Therefore, given the wide variety of research made possible with the APS, it follows that we are all in this together - no single funding source can - or should - bear the total responsibility for instrumenting the APS.

It is important for you to understand that we need to receive proposals before we can act. We are rapidly approaching the time in which it is necessary for proposals to be received, in order that there be enough time to review these proposals, to make decisions on them, to get the funding out - as scarce as it may be - if these proposals are to result in beamlines which will be able to accept the early x-rays from the APS.

The Department of Energy had hoped to spend about $3B this year on various activities in Science and Technology (up from $2.7B last year). That is divided among several different disciplines as shown on slide 1.

Within Energy Research, we have five major activities: Basic Energy Sciences (BES), High Energy Physics and Nuclear Physics, Superconducting Supercollider, Biological and Environmental Research (OHER), Fusion Energy.

Two of these (BES and OHER) are principal supporters for the research which will make use of the APS. I will speak about BES and Roland Hirsch will speak to you about the opportunities in OHER.

The Office of Basic Energy Sciences is composed of the following (slide 2): Materials Sciences (DMS), Chemical Sciences (DCS), Engineering and Geosciences (DE&GS), Advanced Energy Projects (AEP), Energy Biosciences (DEB), and Applied Math.

The operation of User Facilities (slide 3) is included in the DMS and DCS operating budgets. In addition, BES has two other major budget categories: Capital Equipment and Construction which includes Construction of the APS, Accelerator Improvement Projects, General Plant Projects.

The people to contact in BES about funding for beamlines are (slide 4):

Bill Oosterhuis/DMS	(301) 903-3426
Bob Marianelli/DCS	(301) 903-5804
Bill Luth/DE&GS	(301) 903-5829
Roland Hirsch/OHER	(301) 903-3682

The next question is: "will there be any money for beamlines in FY93?" The answer is yes. The Division of Materials Sciences will make some money available to begin the design, if not actual construction of beamlines in FY93, this fiscal year. We are doing this in the face of no increase at all in our FY93 budget because we need to get going on this part of the overall effort. The Construction of the APS is going very well indeed as you will see, but the time to get started on the design and construction of beamlines is now.

How do you go about getting the necessary resources?

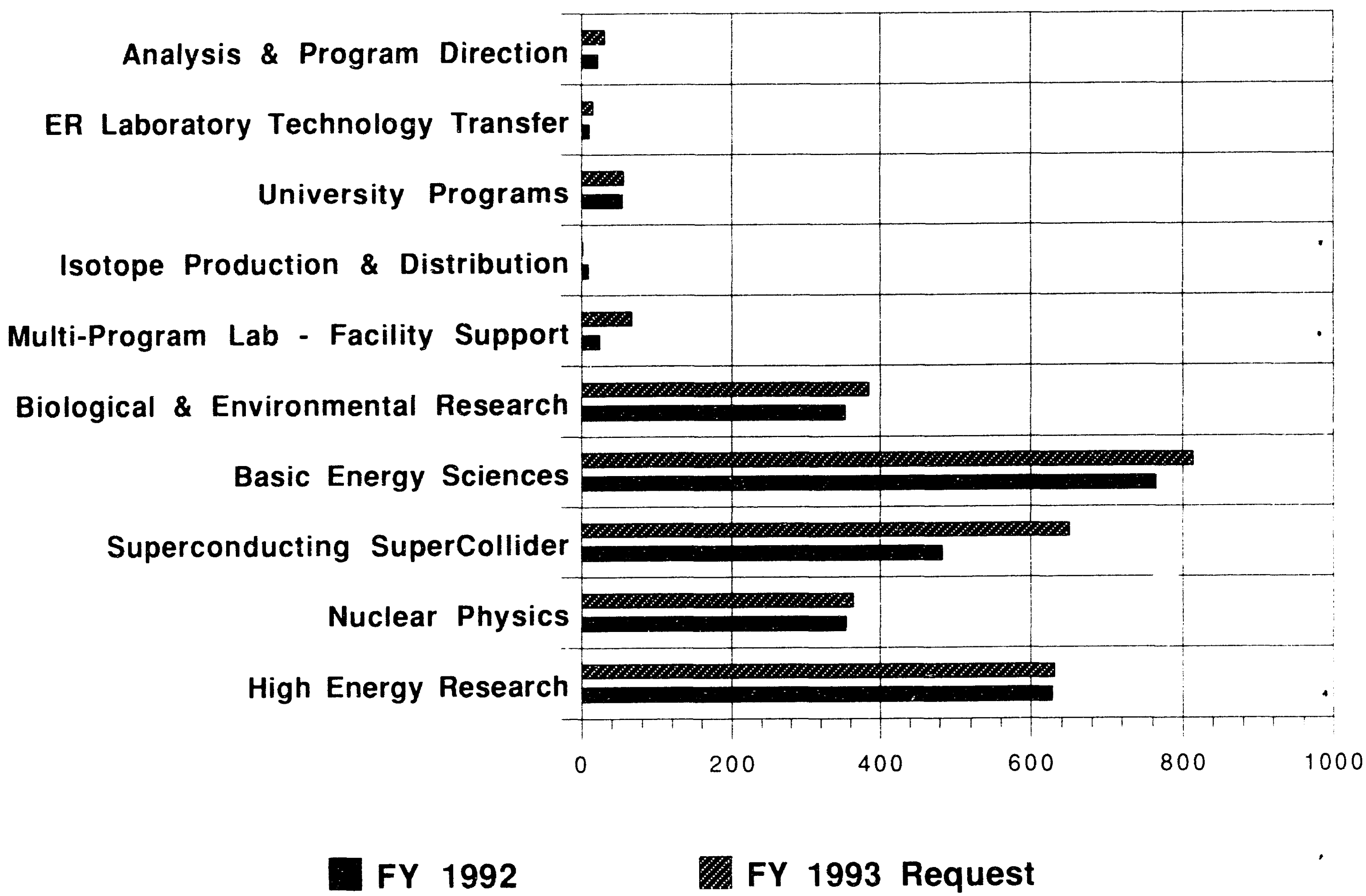
Contact the program people listed above.

Put funding packages together with requests to various funding sources somewhat in proportion to the expected time that will be allocated to various research activities.

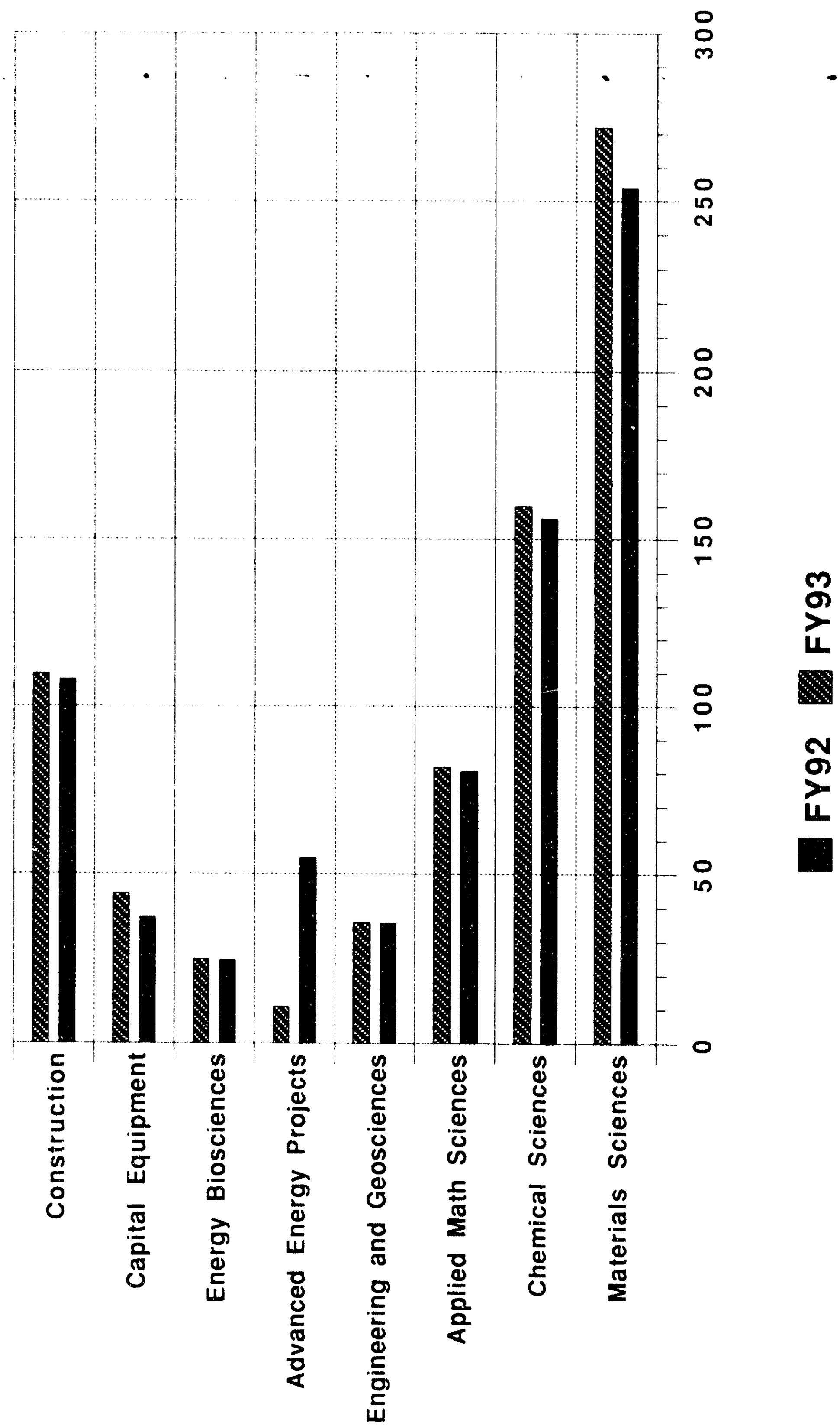
Try to incorporate everything needed for a given beamline, into the same proposal; send the same proposal to each agency with an outline of what you are requesting from each agency.

Cooperate!

DOE Support for Fundamental Science Research ($M)



Basic Energy Sciences ($M)



BASIC ENERGY SCIENCES

FACILITIES SUMMARY

OPERATING EXPENSES

(DOLLARS IN THOUSANDS)

	FY 1990	FY 1991	FY 1992
ONGOING FACILITIES			
NATIONAL SYNCHROTRON LIGHT SOURCE	$ 20,154	$ 22,923	$ 24,400
HIGH FLUX BEAM REACTOR	15,222	22,678	24,400
INTENSE PULSED NEUTRON SOURCE	5,400	6,262	6,800
HIGH FLUX ISOTOPE REACTOR	17,692	28,150	28,500
RADIOCHEMICAL ENGINEERING DEVELOPMENT CENTER	6,850	7,610	7,800
STANFORD SYNCHROTRON RADIATION LABORATORY	10,595	13,413	14,400
MANUEL LUJAN, JR. NEUTRON SCATTERING CENTER	4,437	5,501	5,900
COMBUSTION RESEARCH FACILITY	3,719	4,300	4,700
SUBTOTAL	$ 84,069	$110,837	$116,900
ANS	8,381	11,000	23,600
1-2 GeV	5,548	10,510	19,542
6-7 GeV	9,441	14,332	24,300
SUBTOTAL	23,370	35,842	67,442
TOTAL	$107,439	$146,679	$184,342

DOE Contact People with regard to Beamline Funding

Bill Oosterhuis/DMS	(301) 903-3426
Bob Marianelli/DCS	(301) 903-5804
Bill Luth/DE&GS	(301) 903-5829
Roland Hirsch/OHER	(301) 903-3682

ADVANCES IN SYNCHROTRON RADIATION APPLICATIONS

USING HIGH INTENSITY X-RAYS AT CHESS TO VISUALIZE HOW POLYMERASES COPY GENETIC MATERIALS: 3-D STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE COMPLEXED WITH DOUBLE-STRANDED DNA

Jianping Ding, Raymond G. Nanni, Alfredo Jacobo-Molina, Roger L. Williams, Xiaode Lu, Anqiang Zhang, Chris Tantillo, Arthur D. Clark, Jr., and Edward Arnold

Center for Advanced Biotechnology and Medicine (CABM) and
Rutgers University, Department of Chemistry
679 Hoes Lanes, Piscataway, NJ 08854-5638

1. Features of Synchrotron Radiation that Are Beneficial for Large Molecule Crystallography

Synchrotron radiation (SR) is a unique X-ray source which provides a continuous radiation spectrum of extremely high intensity. Since the cross-section of the circulating electron or synchrotron beam is very small, synchrotron radiation emitted from the beam is restricted to the orbital plane. This natural high collimation ability of very bright SR permits the study of highly detailed structures of complicated biological macromolecules and assemblies with large unit cells where spot sizes must be limited to avoid spatial overlap. For example, in the structure determinations of human rhinovirus 14 (HRV14) (Rossmann et al., 1985; Arnold et al., 1987), Mengovirus (Luo et al., 1987), and numerous crystalline complexes of small molecule antiviral agents with HRV14 (e.g., Smith et al., 1986; Badger et al., 1988; Zhang et al., 1993), synchrotron radiation has played a very important role. The continuous radiation allows for wavelength tunability and, hence, can permit protein crystallographers to solve the phase problem using the anomalous dispersion method by collection of multi-wavelength diffraction data about an absorption edge of an incorporated heavy atom. The use of shorter wavelengths can also extend crystal lifetime via reduced radiation damage of protein crystals. These features associated with SR offer the potential to collect data from very small crystals and allow for more rapid and higher resolution data collection with shorter exposure times than is usually attainable from conventional sources. In addition, the availability of white radiation makes possible studies by the Laue crystallographic method. Entire data sets might be collected from individual crystals with total exposure times on the order of a few seconds. This is especially useful for highly radiation sensitive specimens. Other advantages offered by the Laue photography are that the reflections in a large volume of reciprocal space are sampled simultaneously and that the complication of moving crystal methods are avoided since the crystal is stationary in this method. Time-resolved X-ray diffraction studies are another important field of development in Laue crystallography. The intrinsic pulsed nature of SR also promises a number of exciting developments for protein crystallography.

2. Overall Scheme of Our Synchrotron Experiments

A major purpose of carrying our experiments to synchrotron sources is to collect high quality and high resolution diffraction data which cannot be attained from conventional X-ray sources. A number of phases of preparation are crucial for success of these experiments. The protein samples used for the crystallization must be well prepared and purified. Since different crystallization batches may produce different outcomes, a search procedure should be carried out to distinguish and to classify the crystals according to their quality and size. Depending on the number of crystals to be examined on a given trip, different modes of crystal transportation may be considered.

In various trips to use synchrotron radiation at Cornell High Energy Synchrotron Souces (CHESS), we have utilized facilities at the A1, B2, or F1 stations. The A1 station has a fixed energy of 8 keV (λ=1.55 Å) with a high flux obtained from a 6 pole wiggler. It is mainly used for monochromatic oscillation photography and small angle diffraction. The B2 station supplies a bending magnet white radiation beam for Laue photography with energy tunable from 5 to 40 keV (λ=0.7 - 1.7 Å). The F1 station has a monochromatic and very high flux radiation from 25 pole wiggler with energy tunable from 6 to 25 keV (λ=0.8 - 1.8 Å). It incorporates a BL3 level biohazard facility and its own darkroom and the temperature of the BL3 portion of the station can be adjusted to cold temperatures (~6-10° C) if desired. These features make it very suitable for virus crystallography and small angle scattering. For optimal use of beamtime, the diffraction experiment schedule should be well designed and each of the experimental stations (crystal mounting, camera, darkroom and/or storage phosphor scanner) should be reasonably arranged and continuously manned. Initial diffraction results, such as the appearance of a diffraction pattern and its quality, exposure times, spot shapes and spot overlap, should be carefully assessed to ensure that the proper conditions of preparing crystals and the proper experimental parameters of running the camera have been applied. The best crystals should be studied at optimal times such as i) at the completion of injection and tuning when the beam is at its highest intensity; ii) when soaking conditions have been optimized; and iii) when experimental parameters such as exposure times and oscillation range have been determined. During the data collection, the beam alignment should be checked when i) the wavelength is changed; ii) after a few cycles of successful refills; or iii) anytime a problem is suspected. The X-ray beam position can be checked by exposing a small piece of X-ray sensitive paper (Kodak Linagraph 'pink' paper) mounted on a goniometer head. The position of the subsequent 'burn' pattern with respect to the cross-hairs of the camera telescope or viewing telescope should be monitored. The burn pattern should be taken perpendicular to the X-ray beam direction, if possible, since non-orthogonal views complicate the relationship between the burn pattern and the beam position. In order to get immediate feedback from diffraction experiments, high speed Polaroid film (type 57) can be used to track the quality, diffracting lifetime, and resolution limits of crystals. Since background builds up more rapidly on Polaroid film (complicating the detection of weak diffraction features), spatial resolution is poorer and there is a smaller dynamic range than with conventional film.

Diffraction data sets are brought home in the form of either films or digitized images. Data sets are then processed and analyzed using a modified version of the Purdue oscillation film processing package that has been adapted to run on our host Silicon Graphics workstations (MTOPS: Machine Transportable Programs for Oscillation Processing and Scaling, Kamer and Arnold).

In our recent trips to the CHESS F1 station, the use of storage phosphor image plates (made by Fuji) has led to a significant enhancement in the signal quality of diffraction measurements. Since storage phosphor image plates are more sensitive and have a larger detection area than film, it is possible to use a larger crystal-to-detector distance further for image plate than for film. As a result, the background is lower ($1/r^2$ dependency). The results obtained from using image plates have indicated a significant improvement over those obtained in concurrent experiments using photographic film. In one-third the exposure time relative to X-ray film (4-8 seconds per image plate vs. 16-24 seconds per film), we realized approximately a 0.5 Å enhancement in effective resolution with a better signal-to-noise for the image plate relative to the film. With the shorter exposure times required with image plates, it is possible to collect more useful and higher quality diffraction data sets within a given time allocation on the synchrotron beamline and with limited numbers of crystals of good quality. In addition, since the image plates are reusable, use of image plates reduces tremendously the expenses of synchrotron experiments. On a typical trip to CHESS F1, we used to take 600 exposures on 1800 pieces of films (ABC packs); the total cost was about $5000 (films: $3800, sleeves: $950, chemicals etc.: $200). Instead, we now collect 1800 images on storage phosphors in the same time as 600 exposures on films, costing only about $540 for 45 X 2 = 90 8-mm video tapes (one original set and one backup set).

3. X-Ray Diffraction Studies of Human Viruses and HIV-1 Reverse Transcriptase Using Synchrotron Radiation

In recent experiments, our group has used synchrotron radiation resources at CHESS to study the three-dimensional structures of human rhinovirus 14 complexed with antiviral agents that bind to the capsid (at 3.0 Å resolution) and AIDS virus reverse transcriptase (RT) p66/p51 heterodimer complexed with a double-stranded DNA template-primer and a monoclonal antibody Fab fragment (at 3.0 Å resolution).

3.1 Complexes of Human Rhinovirus 14 with Small Molecule Antiviral Agents

We have been able to solve a number of complexes of HRV14 with small molecule antiviral agents that bind to the capsid. For these studies we have been using the cubic crystal form of HRV14 (**a**=445.1 Å) that diffracts to at least

0.5 Å resolution, and the current results have been analyzed at 3.0 Å resolution. In favorable cases, the compounds can be soaked into the crystals at a concentration that permits imaging of the bound drug and associated conformational changes while retaining isomorphism. Two of the best defined complexes that have recently been solved using data from CHESS are HRV14 complexes with SCH 38057 (Zhang et al., J. Mol. Biol., in press) and SDZ-880-061 (Oren et al., in preparation). SDZ 880-061 was synthesized by chemists at the Sandoz Forschungsinstitut in Vienna, Austria (Rosenwirth et al., in preparation) and is one of the most potent of this class of antivirals against HRV14. It was fascinating to discover that this compound significantly increased the radiation stability of HRV 14 cubic crystals (relative to unsoaked control crystals) when using the CHESS A1 station (λ=1.565 Å). SCH 38057 is a new antiviral compound synthesized by chemists at Schering-Plough that seems to exhibit inhibition potentially via a number of different mechanisms (Rozhon et al., Antiviral Research, in press). The 3 Å resolution electron density maps for both of these complexes have been interpreted in detail and yield a clear interpretation of both the bound antiviral compounds and conformational changes in the viral capsid that accompany drug binding. Each of the compounds causes different conformational changes in VP1 protein. In fact, the conformational changes of the HRV 14 capsid proteins in the SCH 38057 complex are more extensive than those observed in any of the other HRV 14 antiviral complexes reported to date. Overall, these results provide important information regarding both mechanisms of viral inhibition and for further drug design that will take advantage of the three-dimensional structure-activity relationships that being developed.

3.2 Structure of HIV-1 Reverse Transcriptase Complexed with a dsDNA and Fab

The HIV-1 reverse transcriptase (RT) enzyme is responsible for the catalytic transformation of the AIDS virus RNA genome into a linear double-stranded DNA that can be permanently integrated into host cell chromosomes. Currently, HIV-1 RT is the potential therapeutic target of the most widely used treatments for AIDS. HIV-1 RT isolated from virions consists of two subunits, p66 (66 kDa) and p51 (51 kDa). They have the same 440 N-terminal amino acids which constitute the polymerase domain and the remaining 120 C-terminal amino acids of p66 comprise the RNase H domain (Goff, 1990). The structure of the HIV-1 RT/Fab crystals has been solved at 7 Å resolution both for the DNA-containing and non-DNA-containing forms (Arnold et al., 1992). The structure of HIV-1 RT complexed with a non-nucleoside inhibitor nevirapine at 3.5 Å resolution has also been reported by Dr. Thomas Steitz's group at Yale University (Kohlstaedt et al. 1992). Recently our laboratory has independently determined the structure of a ternary complex of HIV-1 RT/Fab/dsDNA at 3.0 Å resolution. We report here some preliminary results about the structure determination of this complex.

Our laboratory has used a variety of approaches to improve and to optimize crystallization of HIV-1 RT, including protein engineering aimed at changing the specific amino acids on the surface, making complexes with antibody fragments, or making complexes with synthetic nucleic acids that mimic template-primer substrates. We have succeeded in obtaining high quality crystals of a ternary complex of the HIV-1 RT p66/p51 heterodimer, a monoclonal antibody Fab fragment (Fab 28), and a dsDNA oligomer that diffract X-rays to 2.8 Å resolution at CHESS (Jacobo-Molina et al. 1991). The dsDNA used for the studies is a complementary 19 base/18 base DNA with a one-base overhang in which the duplex region corresponds in sequence to the 18-base RNA/RNA duplex formed between the primer binding site in the viral RNA genome and the 3' end of tRNA primer. The sequence of the 19-mer is 5'-ATGGCGCCCGAACAGGGAC-3' where the 5'-A forms the one-base overhang. The same crystal form has also been grown without DNA, which also diffracts to 3.5 Å resolution using the CHESS F1 station. A very helpful feature of these crystals is that the DNA-containing crystals and the non-DNA-containing crystals are isomorphous, thus permitting a convenient comparison of the RT structure in the presence and absence of nucleic acid. The HIV-1 RT/Fab/dsDNA crystals belong to space group $P3_212$ with a=168.7 Å and c=220.3 Å, and contain one complex per asymmetric unit.

We have been able to collect entire X-ray diffraction datasets to medium resolution (~ 6 Å, with $I/\sigma(I) > 2$ and overall R_{merge} (I) = 5 - 10 %) from single crystals of the HIV-1 RT/dsDNA/Fab complex using the Xuong-Hamlin Mark II system in our home X-ray laboratory. Those results greatly facilitated the interpretation of heavy atom derivatives and initial structure determination of RT at 7 Å resolution. However, the RT crystals show only a maximum useful resolution of about 4-5 Å using a rotating anode generator, and decay considerably following about 15 hours of exposure. The lower resolution area detector work has been a powerful guide for appropriate conditions to use in the precious time allocated for our synchrotron data collection at CHESS. The high flux at CHESS has permitted us to collect datasets from crystals of the HIV-1 RT/dsDNA/Fab complex at 2.8 Å resolution.

High resolution X-ray diffraction datasets were collected at the CHESS F1 station (λ=0.91 Å). The diffraction data from multiple crystals were processed, merged, and scaled togather using the MTOPS package (Kamer and Arnold, unpublished). The combination of all area detector and synchrotron datasets (4 native and 21 derivative datasets) produced the best electron density maps from MIR/solvent flattening calculations. The datasets were merged using local scaling by resoltuion ranges (Matthews et al., 1975) where the CHESS glycerol native dataset was used as reference. Complete three-dimensional solutions for heavy-atom isomorphous difference Patterson syntheses were generated using both minimum and sum functions in the program VECTORMAP (Williams & Arnold, unpublished). Cross-phased difference Fourier syntheses gave a clear verification of the major sites and revealed additional sites that were initially confirmed using cross-vector searches with known sites as input into VECTORMAP. The initial solution of the heavy atom derivatives at high resolution was provided both by interpretation of difference Pattersons and by difference Fouriers using phases from the low resolution derivative datasets at 7 Å (Arnold et al, 1992). The phases used for locating heavy atom positions derived initially from SIR or MIR calculations, but later corresponded to those improved by solvent flattening. The relative occupancy parameters are on an arbitrary scale. The heavy atom scattering contributions were calculated from appropriate single atom scattering factors even for the heavy-metal cluster derivatives; isotropic thermal parameters of B=20 Å^2 were used and not refined. The parameters used for automatic mask generation during solvent flattening (Wang, 1985) at 3.0 Å resolution were: solvent fraction = 75%, empirical constant S = 0.060, and radius = 7.5 Å (PHASES package, Furey & Swaminathan, 1990). The native dataset was merged from 186 image plates and/or films obtained from 36 crystals with an R_{merge} (I) = 0.13, and has 76903 unique reflections ($I>3\sigma(I)$) to 2.8 Å resolution with a completeness of 88.1%. Secondary structural elements of HIV-1 RT were interpreted using a number of electron density maps calculated based on the MIR phases with resolution limits between 3.5 and 4.0 Å resolution; assignment of connections was facilitated by the recently reported structure of HIV-1 RT complexed with nevirapine (Kohlstaedt et al., 1992). The atomic model has been built using program O (Jones et al., 1991). The most prominent electron density for the DNA corresponds to the sugar-phosphate backbone. The phosphates are particularly pronounced. Interpretation of the Fab28 structure was initially guided by matching the four β-barrel domains of McPC603 (Satow et al., 1986) with the electron density and is being completed based on the sequence of Fab28 (Ferris et al., unpublished). The MIR phased maps were improved with the solvent flattening procedure, but many of the amino acid side-chain densities were still poor. We tried different approaches to combine the initial partial model structure into the MIR phase to improve the experimental map quality. The most successful strategy is to generate the molecular envelope used for solvent leveling by combining the MIR phases with those from a partial atomic model which included only the backbone atoms of the residues with unambiguity. The resulting map showed the improved electron densities in the connection regions and for the side chains where there were weak densities in the maps calculated from MIR phases with the average solvent flattening.

The overall folding of the individual subdomains (named fingers, palm, thumb, and connection) in the polymerase domains of HIV-1 RT is similar, however, their spatial arrangements within the respective monomers are dramatically different, resembling that reported by Kohlstaedt et al. (1992). The structure of the template-primer is a hybrid resembling A-form DNA near the polymerase active site and B-form DNA towards the RNase H active site, with a significant bend at the A-/B-junction. The most numerous interactions of HIV-1 RT and the dsDNA (mainly along the sugar-phosphate backbone) occur with the amino acid residues of the palm, thumb, and fingers subdomains of p66. Highly conserved regions in the p66 palm near the polymerase active site include a β-hairpin that interacts with the primer strand and a loop that interacts with the template strand. These structural elements, together with two α-helices of the p66 thumb, act as a clamp to position the template-primer precisely relative to the polymerase active site. The 3'-hydroxyl of the primer terminus is close to the catalytically essential Asp110, Asp185, and

Asp186 residues at the active site and is in a position for nucleophilic attack on the α-phosphate of an incoming nucleoside triphosphate.

4. References

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POWDER DIFFRACTION WITH SYNCHROTRON X-RAYS

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IMPACT OF POWDER DIFFRACTION METHODS

HYDROGEN STORAGE

Metal hydrides

MAGNETS

Fe-Nd-B

CATALYSIS

Zeolites, clays

CERAMICS

Zirconias

NOVEL MATERIALS

C_{60} fullerenes

SUPERCONDUCTIVITY

High T_cs

BATTERIES/FUEL CELLS

β-aluminas

FERROELECTRICS

$PbTiO_3$ etc.

ELECTRO-OPTICS

N.L.O.s eg. $KTiOPO_4$

BIOMINERALS

Apatites

SYNCHROTRON X-RAY STUDIES OF POLYCRYSTALLINE MATERIALS

HIGH BRIGHTNESS / LOW DIVERGENCE

High resolution powder diffraction

Study of lattice distortions and superlattices

Structure determination from powder data

High intensity studies

Time-resolved studies by energy-dispersive methods

High pressure studies

Milligram powder samples

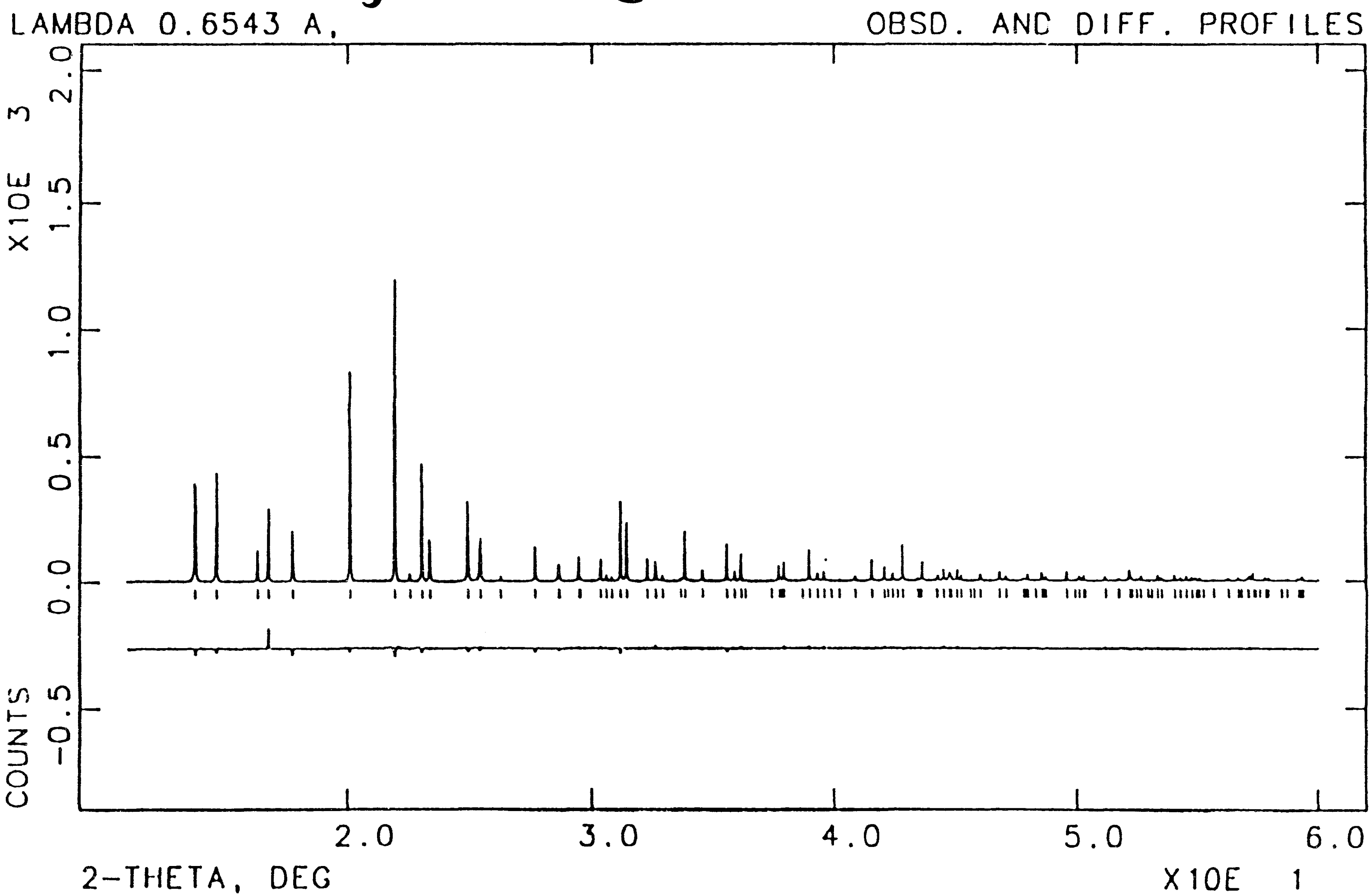
Structures from microcrystals

TUNABILITY

Resonant diffraction studies

High resolution crystal structures from short wavelength data

Rietveld analysis : LiNbO$_3$ (congruent)
(Synch. x-rays)



STEPS IN AB INITIO STRUCTURE DETERMINATION FROM POWDER DIFFRACTION DATA

(i) Unit Cell Determination

Auto indexing
Selected area electron diffraction

(ii) Pattern Decomposition

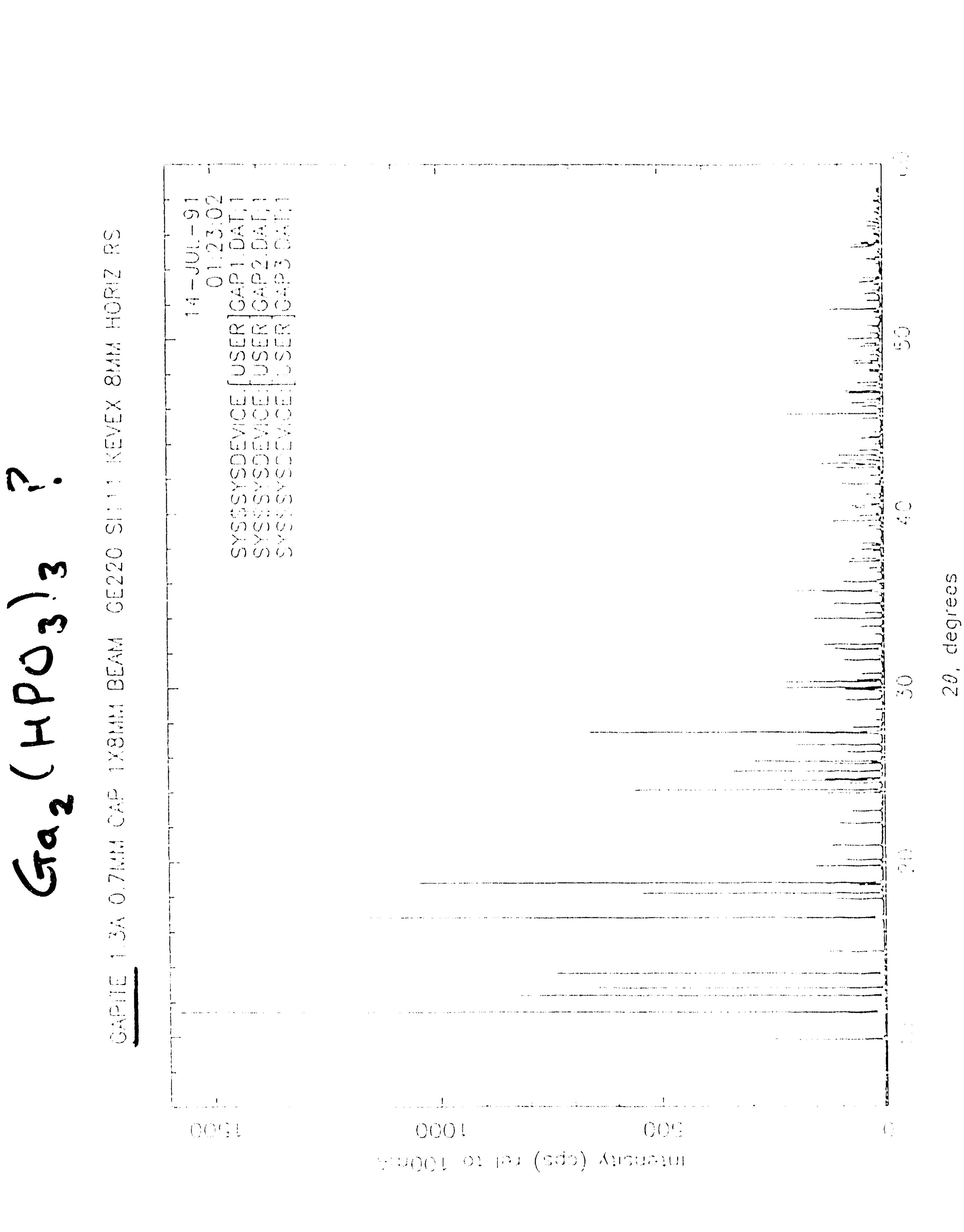
Yields I_{hkl} values and (?) space group
(Pawley and Le Bail methods)

(iii) Phase Determination

Patterson and Direct Methods

(iv) Structure Refinement

Rietveld method


Ga2(HPO3)3 ?
GAPIE 1.3A 0.7MM CAP 1X8MM BEAM GE220 SI111 KEVEX 8MM HORIZ RS
14-JUL-91
01:23:02
SYS$SYSDEVICE:[USER]GAP1.DAT;1
SYS$SYSDEVICE:[USER]GAP2.DAT;1
SYS$SYSDEVICE:[USER]GAP3.DAT;1
2θ, degrees
20
30
40
50
Intensity (cps) rel to 100mA
0
500
1000
1500

STRUCTURE SOLUTION OF GAPHI

Synthesis: $GaCl_3 + H_3PO_3$ Reflux for 24hrs.

Synchrotron X-ray powder diffraction collected at Brookhaven National Lab.
$\lambda = 1.2995$Å, 2θ range 15 - 100°

Indexing: Treor Autoindexing Program from 26 2θ values measured using a Scintag Pad-V powder diffractometer. Systematic absences indicated possible space groups $P2_1$, Pm or $P2_1/m$. SHG was approx 1.5 times that of quartz ==> non centrosymmetric structure.

a = 8.1384(2), b = 10.0388(2), c = 7.7024(2),
β = 111.58(1), Z=2.

Space group: $P2_1$

Structure solution: Intensities for 551 reflections were extracted from the profile using the Le Bail method. 19 of these reflections were rejected as having zero intensity.

Fs for 532 reflections were input into the SHELXS - 86 direct methods program.

17/6/91.

Russ $GaCl_3 + H_3PO_3$

200MHz ≡ 81.020 for ^{31}P

CP/MAS

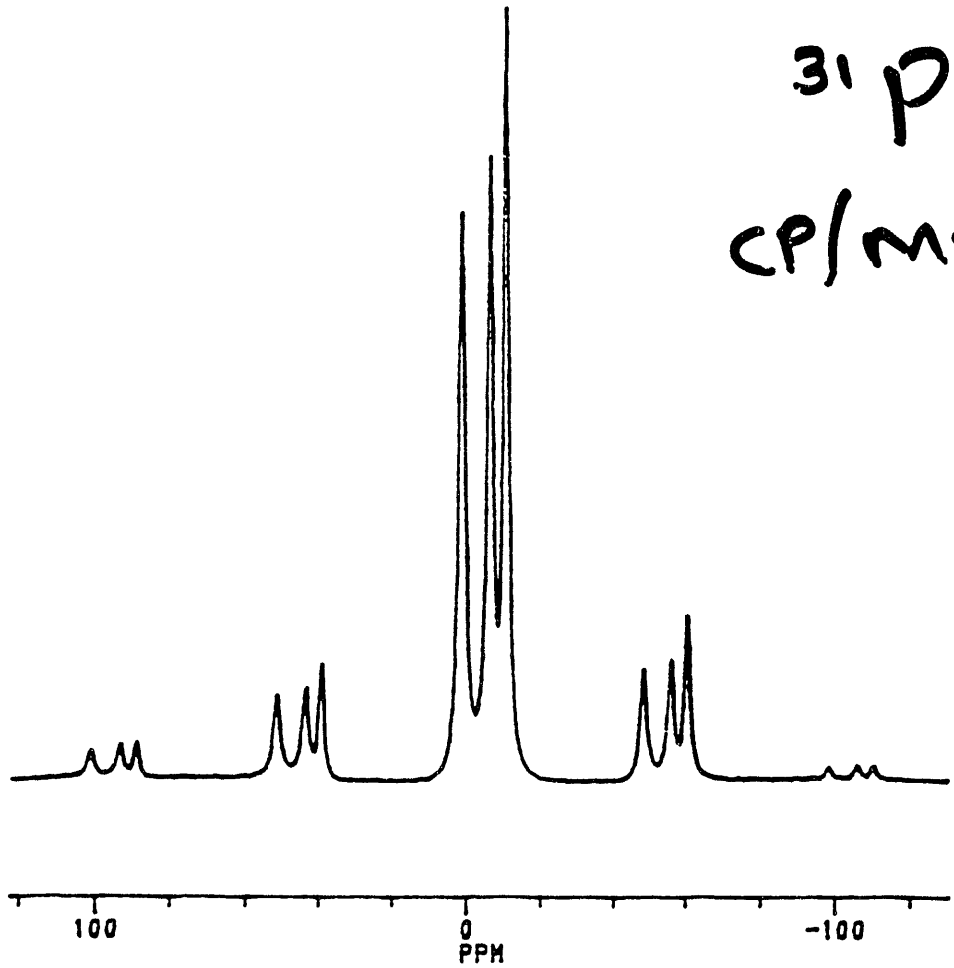
1M = contact time

15s = recycle time

NS = 100

Rotor speed = 4030Hz

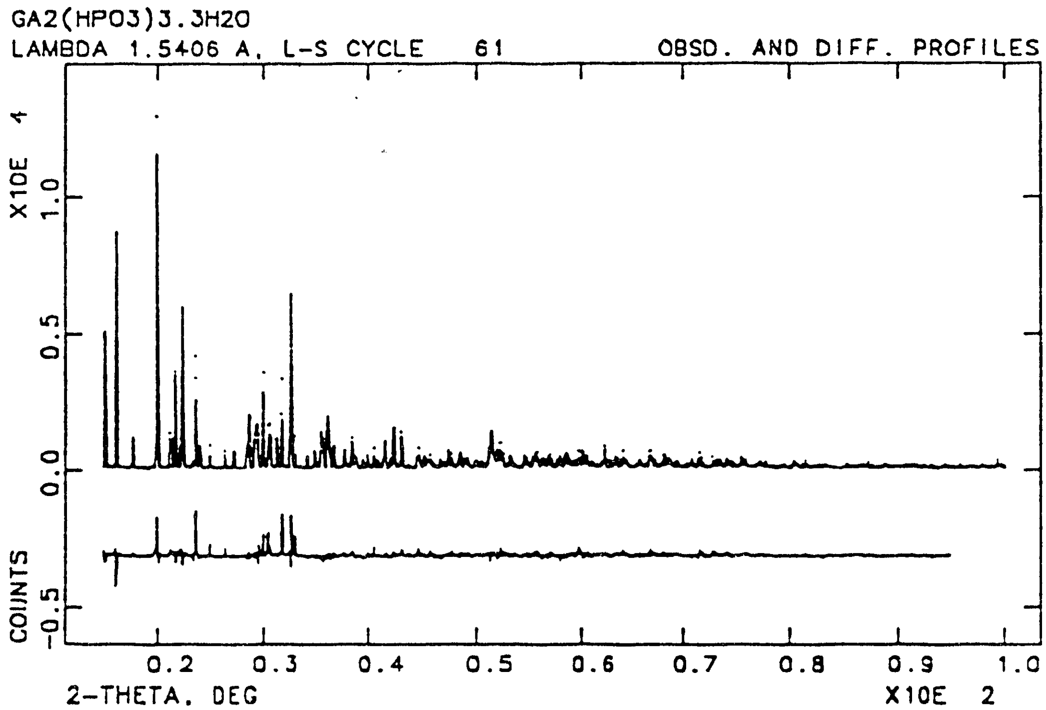
Shifts = .928ppm
-6.6 "
-10.8 "



^{31}P CP/MAS

Structure solution involved refinement of 151 E values (E > 1.2), using 1486 unique TPR and 168 negative Quartets.

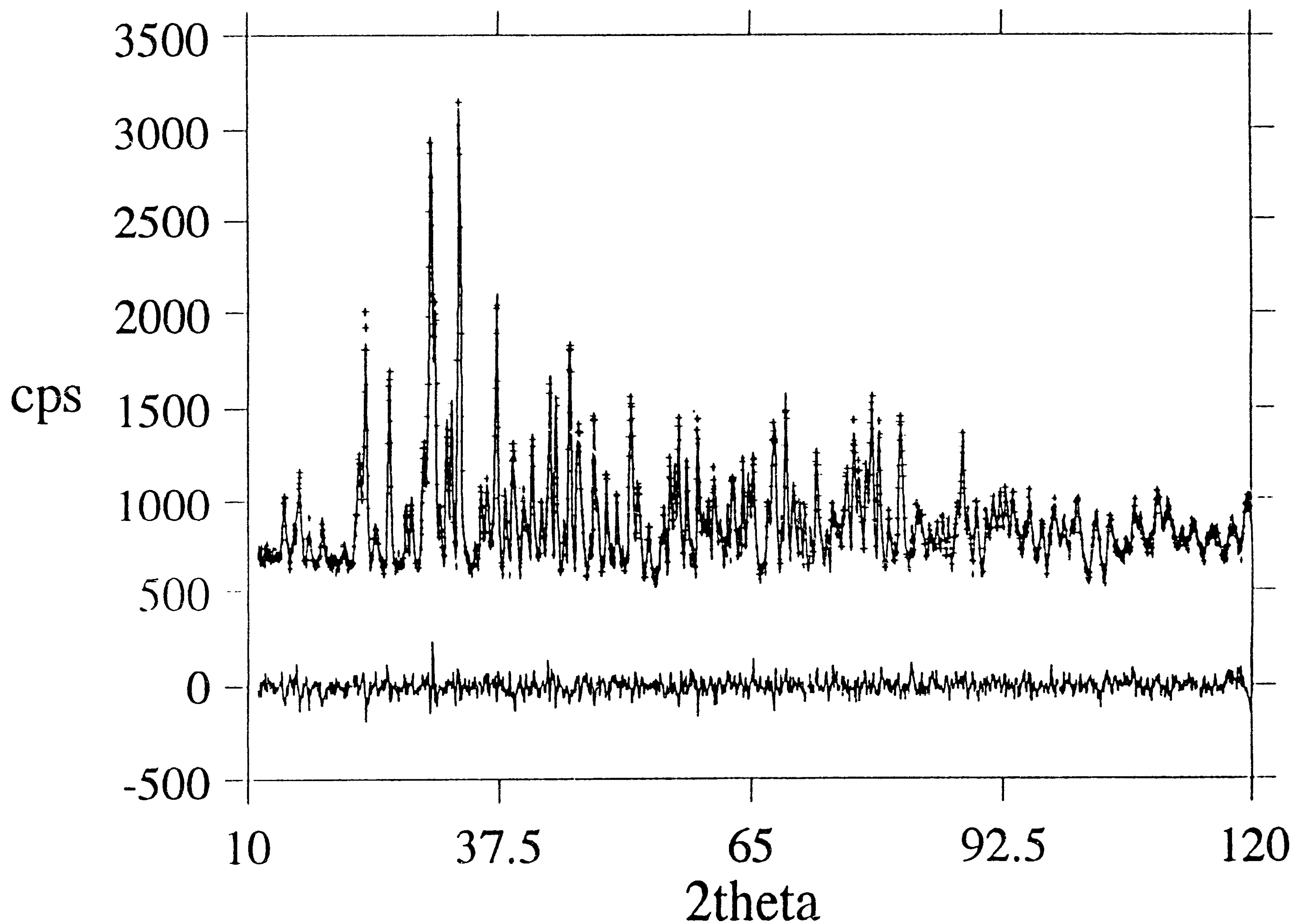
Gallium, phosphorus and most oxygen atoms were located at this stage, following refinement and difference Fourier calculations..



Neutron Diffraction (with a deuterated sample) was used to find remaining atoms and confirm the stoichiometry as $Ga_2(HPO3)3.4H2O$.

Conclusion: Structure refined with 29 atoms in the asymmetric unit, 118 structural parameters!

Final Observed (+), Calculated (—) and Difference Profiles for $Ga_2(HPO_3)_3.4H_2O$



Final Atomic Coordinates for $Ga_2(HPO_3)_3.4H_2O$

Ga(1)	0.0226(10)	0.3523(7)	0.0645(11)
Ga(2)	0.3766(9)	0.0757(7)	0.5854(11)
P(1)	0.3439(12)	0.3714(12)	0.4556(13)
P(2)	-0.0103(12)	0.0776(11)	0.2485(14)
P(3)	-0.0859(14)	0.6313(11)	0.2189(15)
O(1)	0.2586(12)	0.3682(11)	0.2396(14)
O(2)	-0.0497(13)	0.4829(10)	0.2035(14)
O(3)	-0.0568(14)	0.2223(10)	0.2059(15)
O(4)	0.1242(12)	0.2071(10)	-0.0378(15)
O(5)	0.0906(14)	0.4827(9)	-0.0849(16)
Ow(6)	-0.2140(15)	0.3406(10)	-0.1256(13)
O(7)	0.4555(13)	0.2595(10)	0.5453(14)
O(8)	0.1954(13)	0.0480(10)	0.3444(14)
O(9)	-0.2162(12)	0.6551(10)	0.3096(13)
O(10)	0.5391(13)	0.0007(9)	0.4861(14)
Ow(11)	0.5698(14)	0.0915(10)	0.8478(15)
Ow(12)	0.3224(12)	-0.1031(9)	0.6751(13)
Ow(13)	0.4925(15)	0.1676(11)	0.1586(16)
Dp(1)	0.2089(11)	0.3938(8)	0.5259(11)
Dp(2)	-0.0860(13)	0.0425(10)	0.3821(14)
Dp(3)	0.0843(14)	0.6729(12)	0.3454(14)
Dw(61)	-0.2550(15)	0.4054(13)	-0.2428(16)
Dw(62)	0.3010(16)	0.7752(11)	0.1647(16)
Dw(111)	0.6701(19)	0.0309(14)	0.8855(19)
Dw(112)	0.5376(15)	0.1131(11)	0.9477(16)
Dw(121)	0.4005(15)	-0.1797(11)	0.7265(17)
Dw(122)	0.2216(13)	-0.1039(11)	0.7159(14)
Dw(131)	0.3614(17)	0.1900(14)	0.1081(18)
Dw(132)	0.5187(20)	0.1127(14)	0.2653(26)

Final Bond Distances (Å) for $Ga_2(HPO_3)_3.4H_2O$

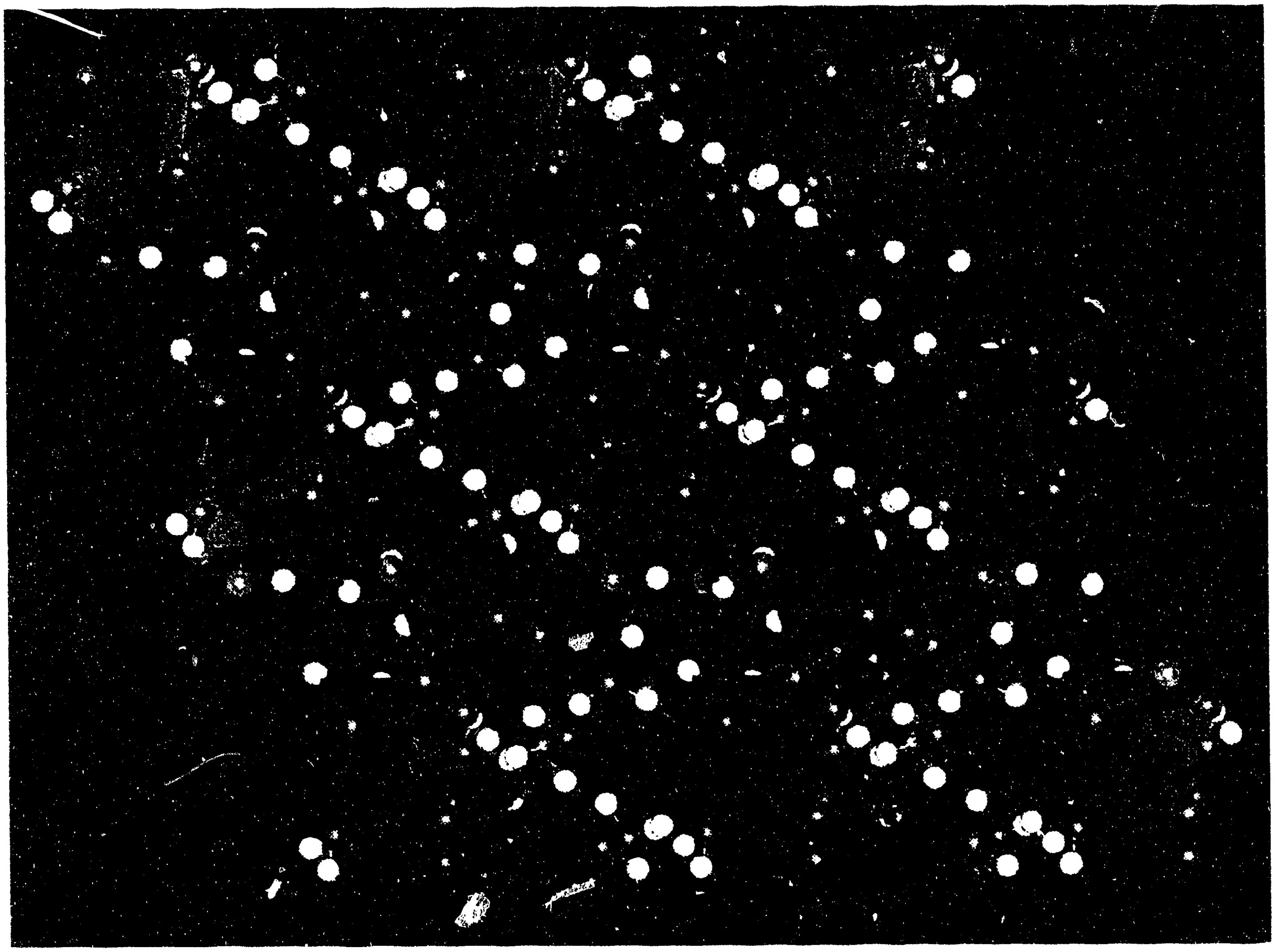
Ga(1)	—	O(1)	1.899(12)	Ga(2)	—	O(7)	2.011(12)
Ga(1)	—	O(2)	1.912(13)	Ga(2)	—	O(8)	1.915(12)
Ga(1)	—	O(3)	1.949(12)	Ga(2)	—	O(9)	1.932(11)
Ga(1)	—	O(4)	1.971(13)	Ga(2)	—	O(10)	1.899(12)
Ga(1)	—	O(5)	1.946(12)	Ga(2)	—	Ow(11)	2.056(13)
Ga(1)	—	Ow(6)	1.942(14)	Ga(2)	—	Ow(12)	2.027(12)

P(2)	—	O(3)	1.505(15)	P(1)	—	O(1)	1.546(13)
P(2)	—	O(5)	1.520(14)	P(1)	—	O(7)	1.448(14)
P(2)	—	O(8)	1.583(14)	P(1)	—	O(10)	1.572(15)
P(2)	—	Dp(2)	1.418(15)	P(1)	—	Dp(1)	1.402(11)

P(3)	—	O(2)	1.530(15)
P(3)	—	O(4)	1.514(14)
P(3)	—	O(9)	1.479(14)
P(3)	—	Dp(3)	1.428(14)

Ow(6)	—	Dw(61)	1.060(14)	Ow(11)	—	Dw(111)	0.970(15)
Ow(6)	—	Dw(62)	0.929(13)	Ow(11)	—	Dw(112)	0.921(14)

Ow(12)	—	Dw(121)	0.981(12)	Ow(13)	—	Dw(131)	1.013(15)
Ow(12)	—	Dw(122)	0.975(13)	Ow(13)	—	Dw(132)	0.944(17)



$Ga_2(HPO_3)_3.4H_2O$

Some Examples of *Ab Initio* Structure Determinations from Synchrotron X-ray Powder Data.

Compound	Space Group	No. of Atoms in Asymmetric Unit
α-$CrPO_4$	Imma	8
I_2O_4	$P2_1/c$	6
$Al_2Y_4O_9$	$P2_1/c$	15
$MnPO_4.H_2O$	C2/c	6
PbC_2O_4	P1	7
Clathrasil, Sigma-2	$I4_1/amd$	17
$LaMo_5O_8$	$P2_1/a$	14
BeH_2	Ibam	4
UPd_2Sn	Pnma	4
$C_5H_{11}NO_2$	$Pna2_1$	19
$NaCD_3$	I222	10
$BaBiO_{2.5}$	$P2_1/c$	5
$(VO)_3(PO_4)_2.9H_2O$	$P2_1/n$	13 non-H
$CuPt_3O_6$	$Pn2_1m$	10
$Ga_2(HPO_3)_3.4H_2O$	**$P2_1$**	**29 incl. H**

CO_2 REFORMING OF NATURAL GAS OVER $Ln_2Ir_2O_7$

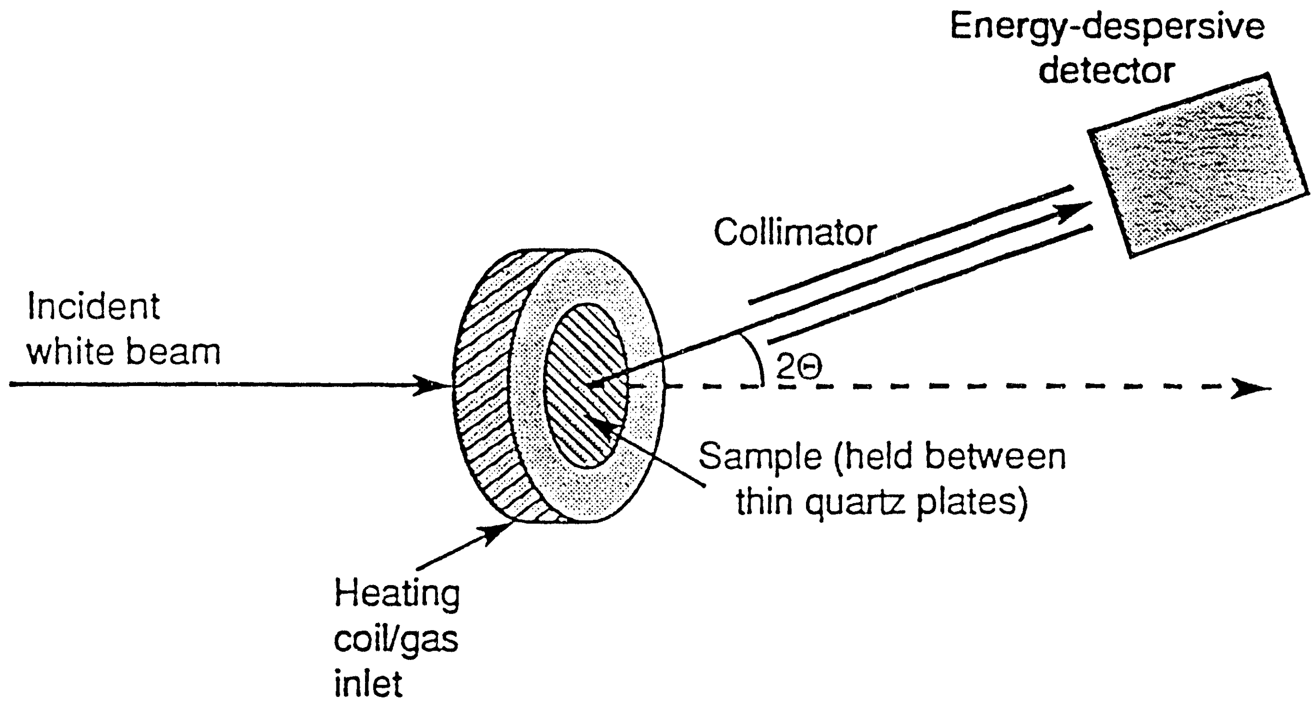
$$CO_2 + CH_4 \text{ ----------> } 2CO + 2H_2$$

Up to 90% conversion with ~98% selectivity

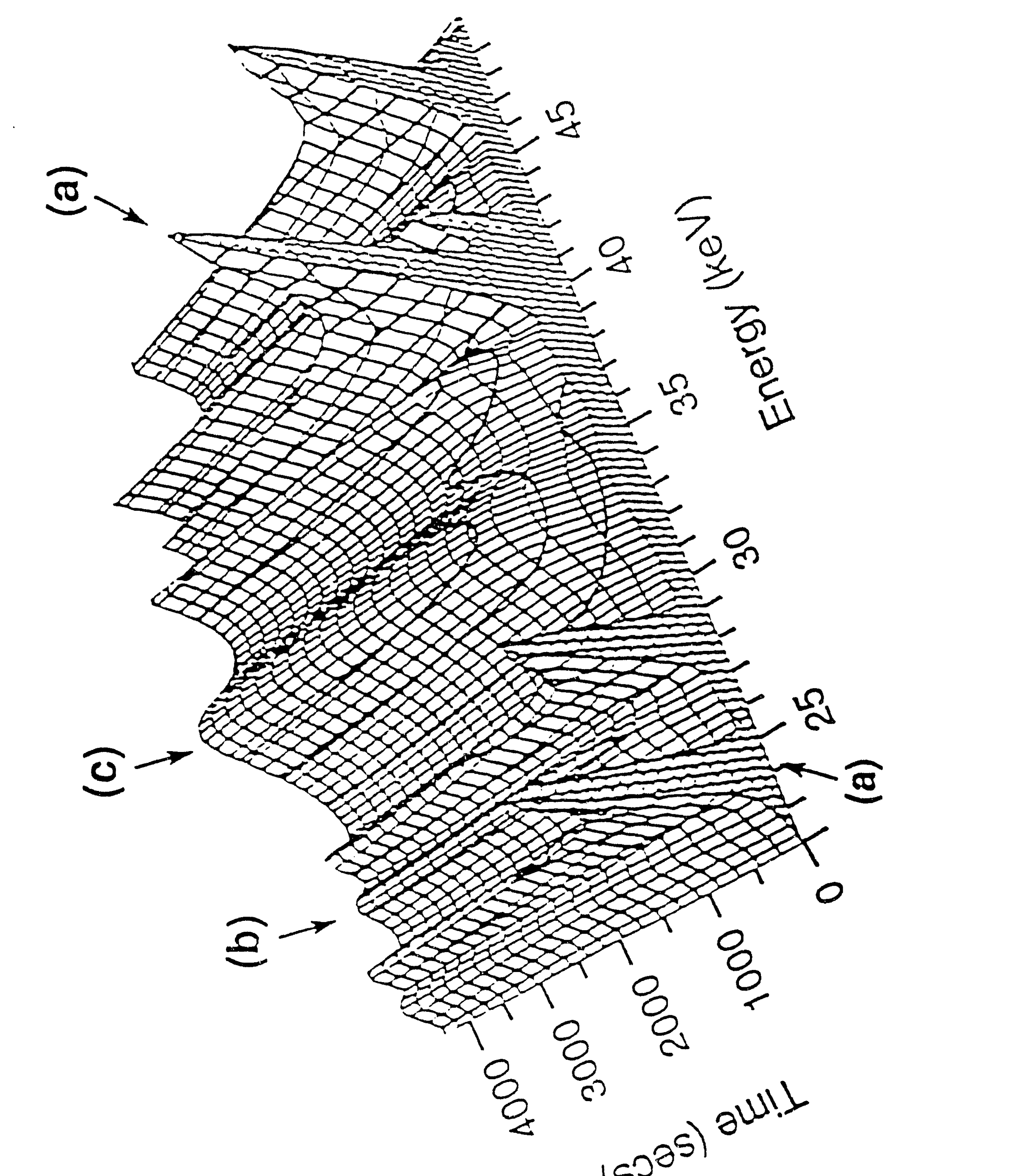
Energy-dispersive X-ray diffraction with synchrotron radiation shows that decomposition takes place according to:

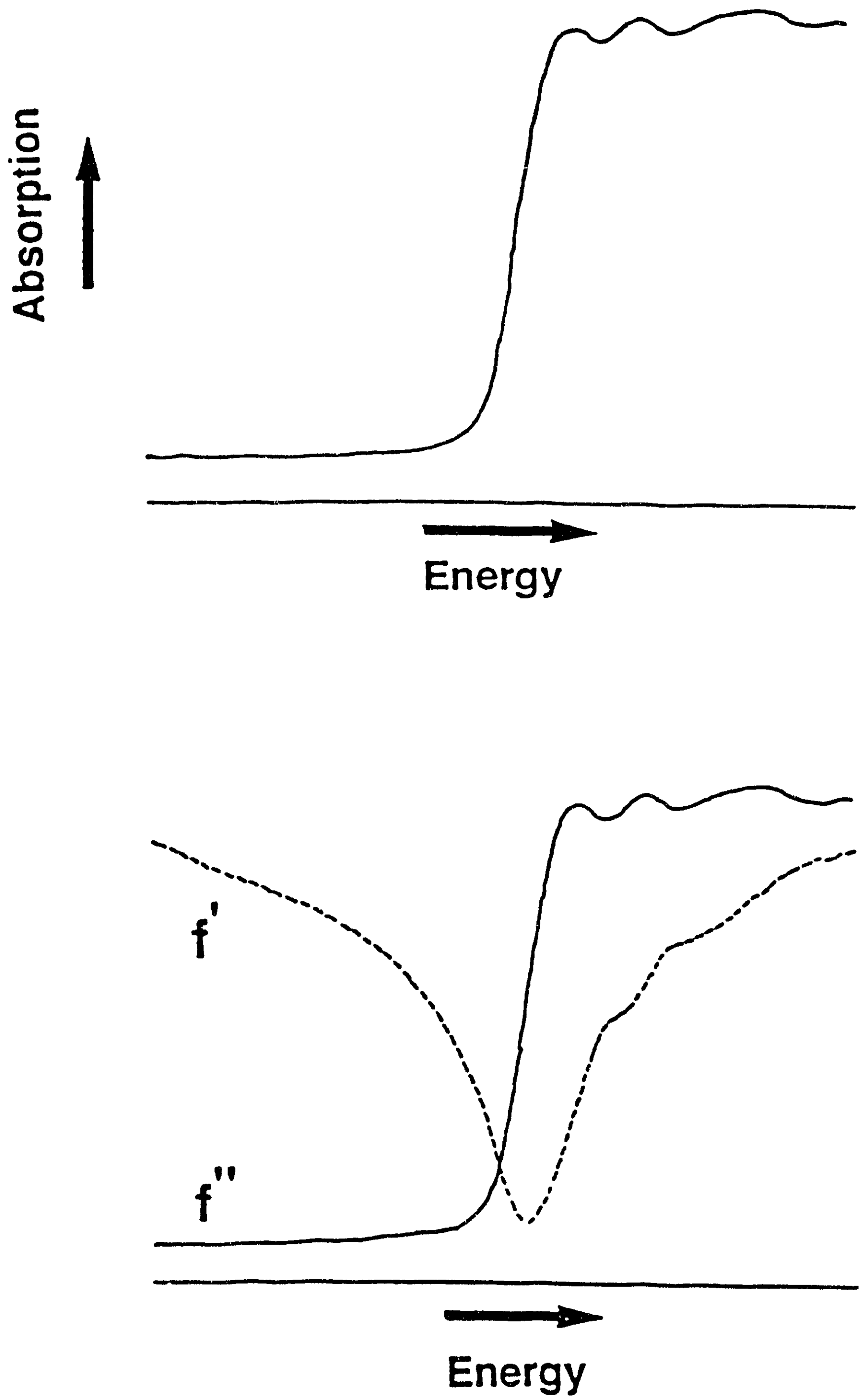
$$Ln_2Ir_2O_7 \text{ ---> } Ln_2O_3 + Ir + O_2$$

Supported Ir is the active catalyst



Cheetham-Shell-9/3/92-amk-02#858-1


(a)
(c)
(b)
(a)
Energy (keV)
25
30
35
40
45
Time (secs)
0
1000
2000
3000
4000



The relationship between absorption, f ' and f ''

SOME APPLICATIONS OF RESONANT X-RAY DIFFRACTION

(i) Neighbouring element contrast;
e.g. $FeCo_2(PO_4)_2$

$f^o{}_{Fe^{2+}}$ = 24 electrons, f' = -7.8 e^-
$f^o{}_{Co^{2+}}$ = 25 electrons

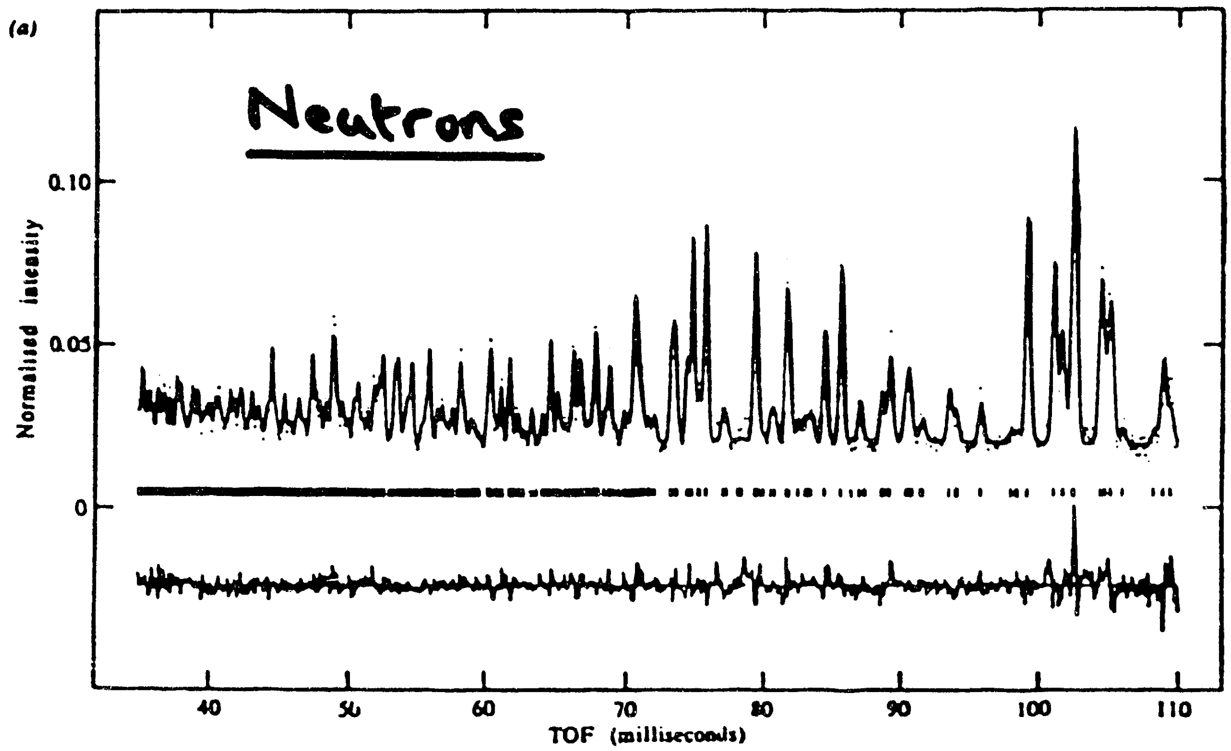
(ii) Valence contrast in mixed valence cpds.
e.g. $\alpha-Fe_2PO_5$ ($Fe^{II}Fe^{III}PO_5$)

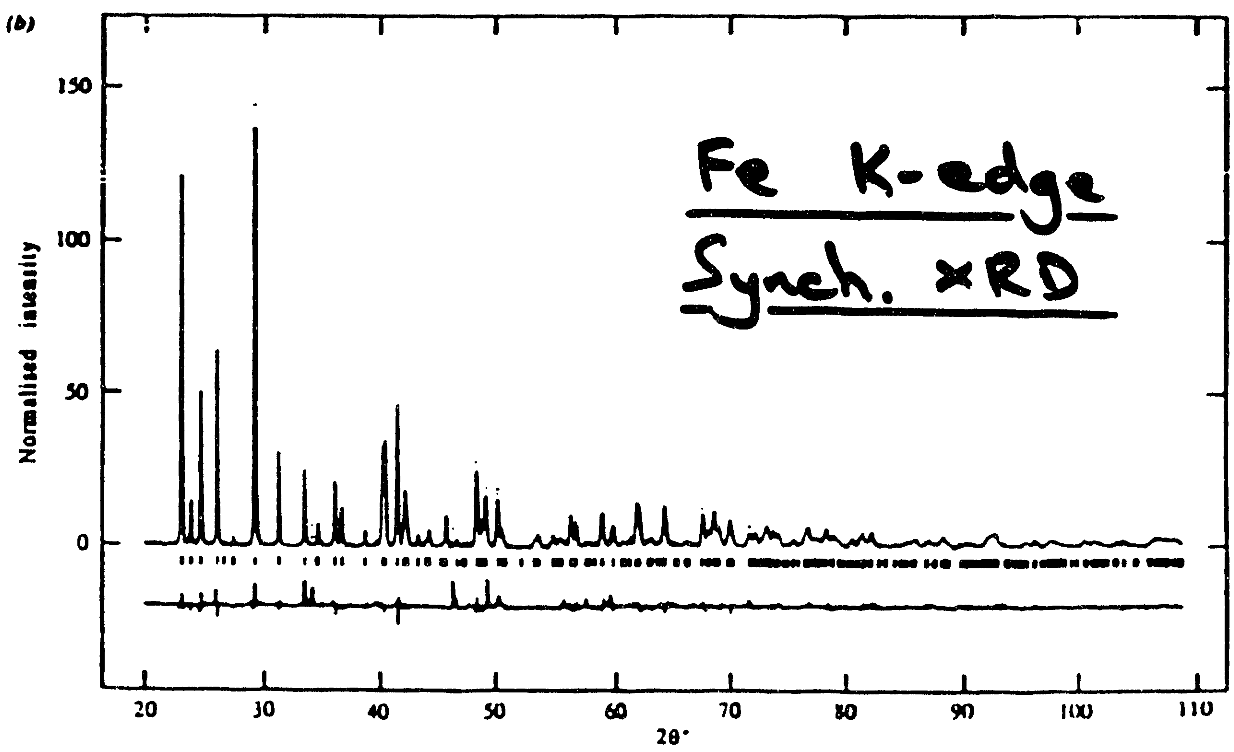
(iii) Multiple site occupancies in zeolites, high T_cs etc.

(iv) Site selective XANES studies

(v) Structure determination from powder data

Co2Fe(PO4)2





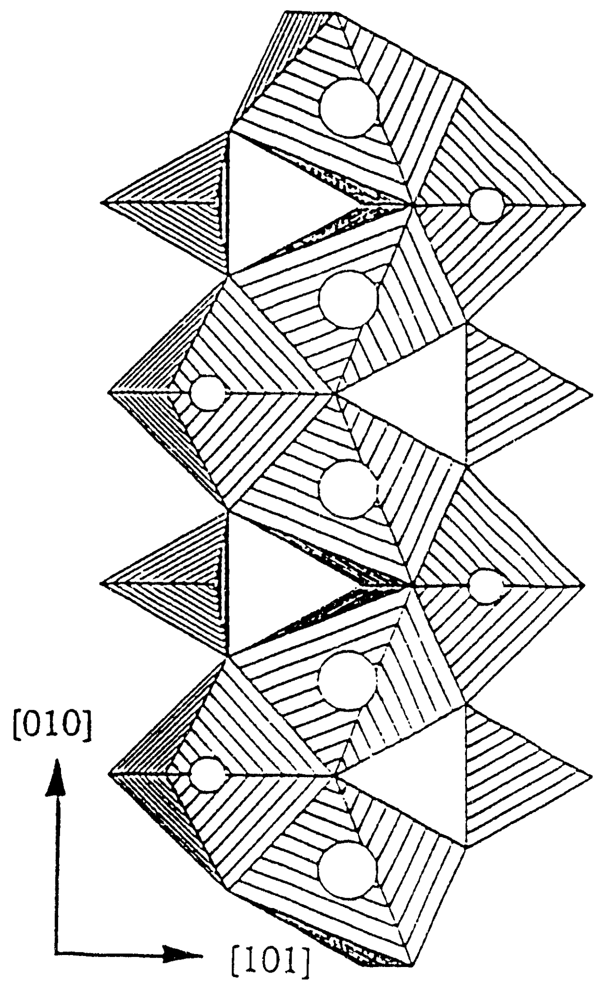
The observed (dots) and calculated (continuous line), and difference profiles for $Co_2Fe(PO_4)_2$ with: (*a*) time-of-flight neutron and (*b*) resonant X-ray powder diffraction. Reflection positions are shown as bars.

Occupancy of Fe by neutron and resonant X-ray powder diffraction in $Co_2Fe(PO_4)_2$*.

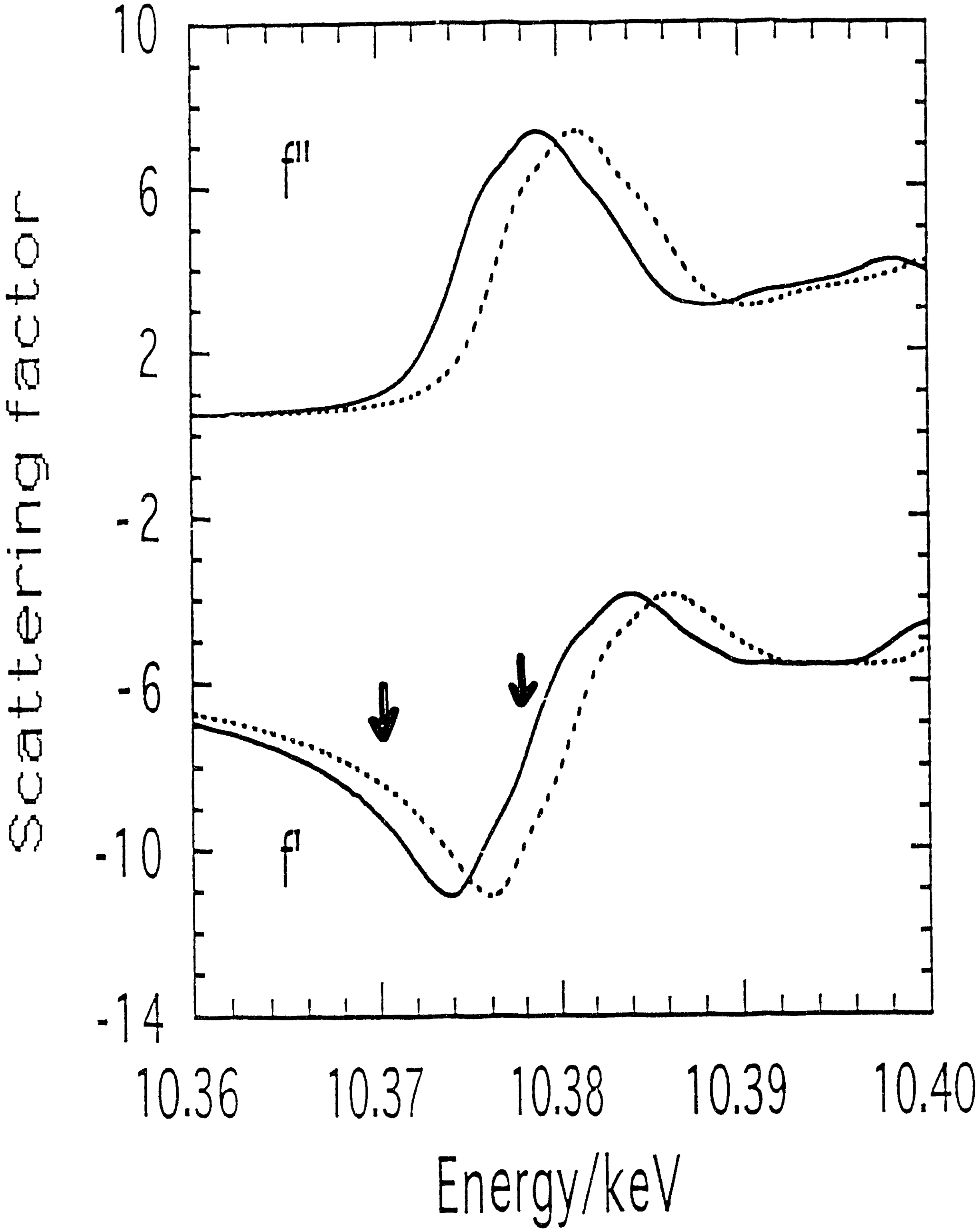
	Fe Occupancy	
Site	M(1)	M(2)
Statistical Distribution	1/3	1/3
TOF Neutrons	0.251(4)	0.498(8)
X-rays Fe *K*-edge	0.243(5)	0.514(10)
Multiplicity	4	2
Coordination	5	6

* Overall composition constrained to the chemical formula.

α- Fe_2PO_5



The effect of oxidation state



VALENCE CONTRAST IN Fe_2PO_5

Resonant X-ray diffraction:
The Fe^{2+} *K*-edge:

M(1) site $f' = -9.74(5)$,
M(2) site $f' = -8.04(7)$

The Fe^{3+} edge:

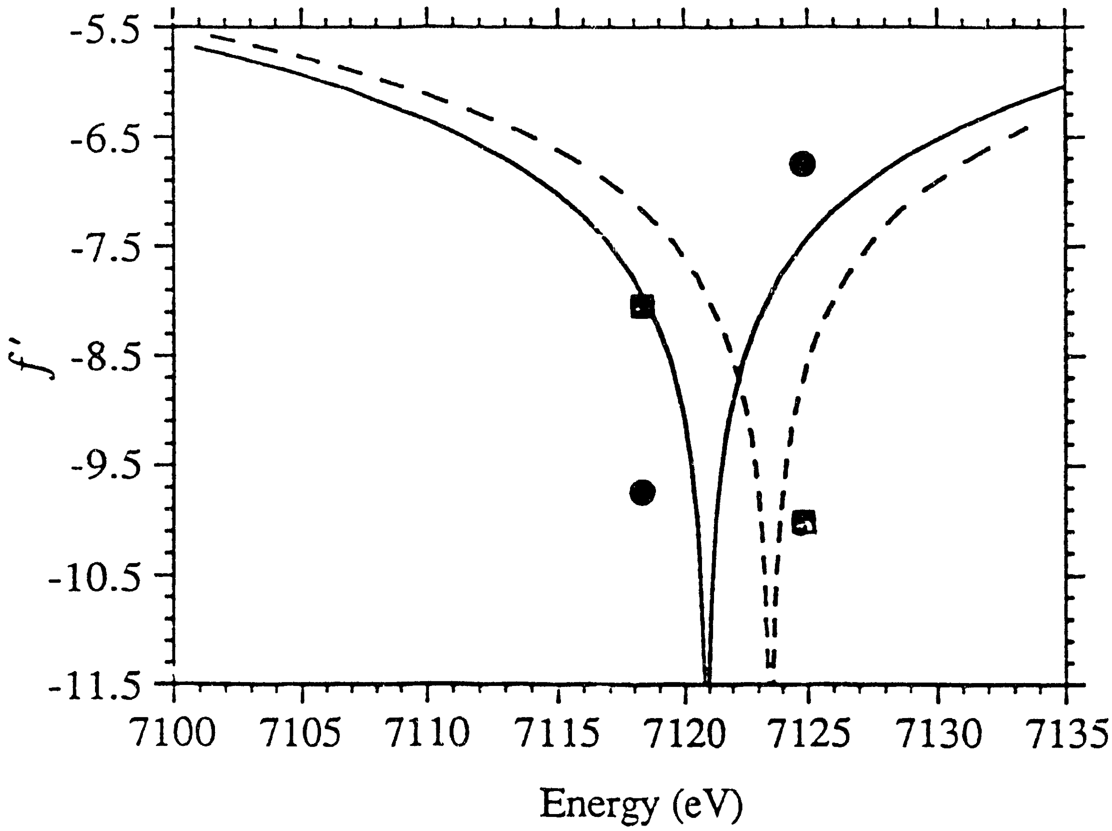
M(1) site $f' = -6.75(11)$
M(2) site $f' = -10.01(17)$

Neutron diffraction has been used to solve the magnetic structure and refine values for the magnetic moment at each iron site:

$M(1)=3.89(3)\mu B$
$M(2)=4.22(3)\mu B$

Both diffraction experiments confirm the presence of Fe^{2+} at M(1) and Fe^{3+} at M(2), and are in agreement with valence bond calculations:
$\Sigma s M(1)=2.077(3)$, $\Sigma s M(2)=2.997(7)$
(based upon the room temperature crystal structure)

α-Fe_2PO_5



● Fe^{2+}

■ Fe^{3+}

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Simon Clarke

—

Richard Jones
John Thomas

—

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SHELL

DAFS: A NEW X-RAY STRUCTURAL TECHNIQUE USING REAL PHOTONS AND VIRTUAL PHOTOELECTRONS

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1. Synopsis

This talk described the work that my collaborators and I have done over the past two years developing and applying the new x-ray technique DAFS. Most of the material presented in the talk has been published in the three references listed below. The essential physical idea behind DAFS is that causality and unitarity require the diffracted intensities to have the same fine structure versus photon energy as x-ray absorption. Consequently, DAFS unifies diffraction and XAFS sensitivities into a single technique, and thereby provides enhanced sensitivities for special applications.

2. References

1. H. Stragier, J.O. Cross, J.J. Rehr, L.B. Sorensen, C.E. Bouldin and J.C. Woicik, "Diffraction Anomalous Fine Structure: A New X-Ray Structural Technique," *Physical Review Letters* **69**, 3064 (1992).

2. C.E. Bouldin, J.C. Woicik, H. Stragier, J.O. Cross, J.J. Rehr and L.B. Sorensen, "Diffraction Anomalous Fine Structure: XAFS with Virtual Photoelectrons," *Japanese Journal of Applied Physics* **32**, 198 s2 (1993).

3. D.J. Tweet, K. Akimoto, I. Hirosawa, T. Tatsumi, H. Kimura, J. Mizuki, L.B. Sorensen, C.E. Bouldin and T. Matsushita, "Structural Study of the $Si/B\sqrt{3}\times\sqrt{3}R30^{\circ}/Ge_x Si_{1-x}$ Interface by Spatially Selective Diffraction Anomalous Fine Structure (DAFS)," *Japanese Journal of Applied Physics* **32**, 203 s2 (1993).

DAFS: A NEW X-RAY STRUCTURAL TECHNIQUE

HANS STRAGIER	THESIS *	UNIVERSITY
JULIE CROSS	THESIS *	OF
JOHN REHR	THEORY	WASHINGTON

CHARLES BOULDIN — NIST
JOE WOICIK

B/GeSi:
DOUGLAS TWEET — NEC
JUN'ICHIRO MIZUKI
KOICHI AKIMOTO
ICHIRO HIROSAWA
TORU TATSUMI

TADASHI MATSUSHITA — PHOTON FACTORY

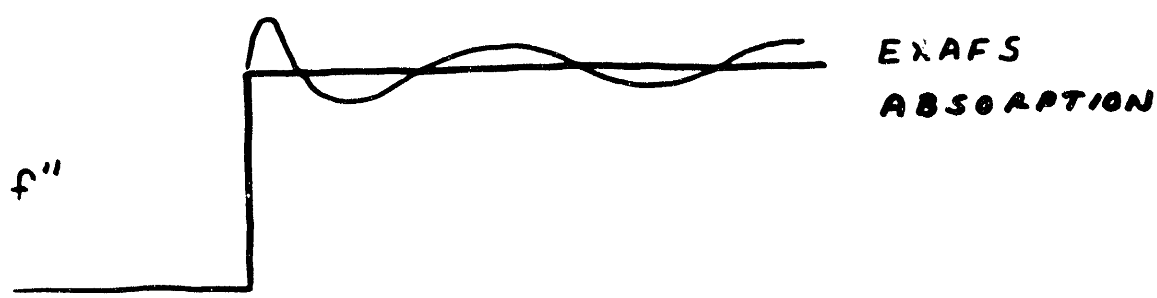
DATA: NIST X23A2 NSLS

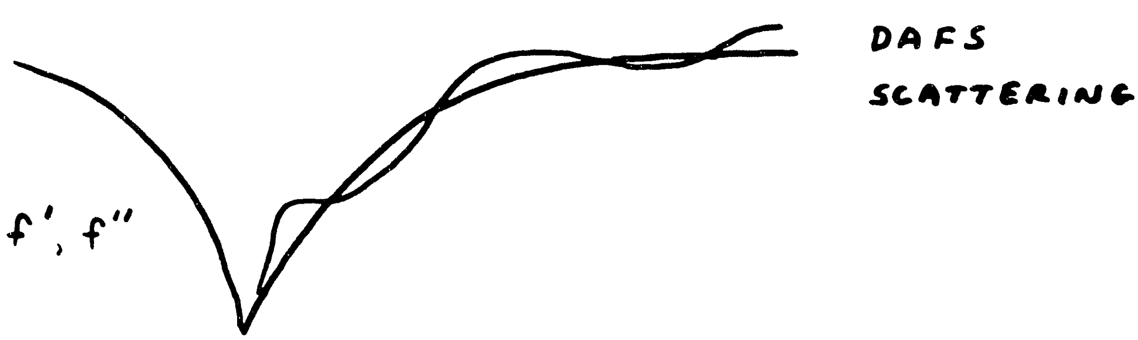
B/GeSi:	NEC	9C	PHOTON
	PF	16A	FACTORY

DAFS: DIFFRACTION ANOMALOUS FINE STRUCTURE

IDEA: HIGH PRECISION MEASUREMENTS OF THE SCATTERING INTENSITY PROVIDE THE SCATTERING CHANNEL f', f'' ANALOGS OF THE f'' ABSORPTION CHANNEL FINE STRUCTURE OBSERVED IN EXAFS

$f' \longleftrightarrow f''$: KRAMERS-KRONIG TRANSFORM PAIR





DAFS UNIFIES XAFS AND XRD INTO A SINGLE TECHNIQUE THAT USES THE FULL FOUR-VECTOR, $(\vec{p}, E)$, NATURE OF THE PHOTON (CAN ALSO USE $\vec{S}$)

EXAFS ONLY USES E

XRD ONLY USES $\vec{p}$

AXRD USES $\vec{p}$ AND A FEW E's

DAFS USES $\vec{p}$ AND E

DIFFRACTION ⇒ LONG-RANGE ORDER

EXAFS ⇒ SHORT-RANGE ORDER

COMBINE THEM TO GET BOTH!

EXAFS: CHEMICALLY SPECIFIC, SRO

AXRD: CHEMICALLY SPECIFIC, LRO

DAFS: CHEMICALLY SPECIFIC, LRO & SRO

DAFS PROVIDES: CHEMICAL SELECTIVITY
NEIGHBOR DISTANCES
NEIGHBOR FRACTIONS
NEIGHBOR DISORDERS
SPATIAL SELECTIVITY
SITE SELECTIVITY
VALENCE, ORBITAL SENSITIVITY

1) SPATIAL SELECTIVITY

CAN SEPARATE COMPONENTS WITH DIFFERENT $\vec{Q}$'s

STRAINED LAYERS	InGaAs
MIXED POWDERS	Cu
SURFACE MONOLAYERS	
SURFACE / BURIED INTERFACE RECONSTRUCTIONS	Ge B Si

2) SITE SELECTIVITY

SCATTERING AMPLITUDE IS A LINEAR COMBINATION OF THE INEQUIVALENT SITE AMPLITUDES => CAN SEPARATE INEQUIVALENT SITES

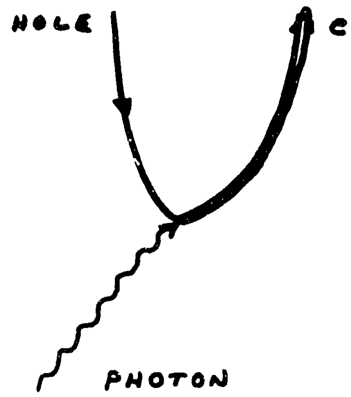
BULK SAMPLES	123 SUPERCONDUCTORS
	SPINELS Co

3) VALENCE AND ORBITAL SENSITIVITY

⟶ NEAR EDGE REGION

THE COMPLEMENTARITY:

EXAFS

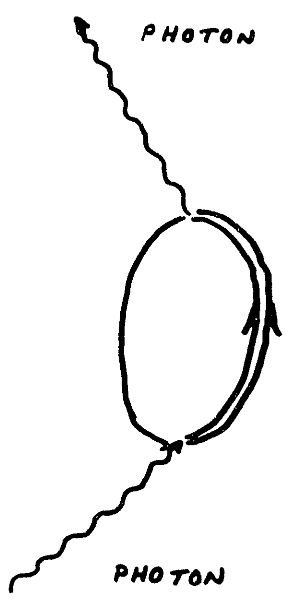


$(\vec{p} \cdot \vec{A})$

REAL ELECTRON IN THE FINAL STATE
WAVEFUNCTION MODULATED BY THE NEIGHBORING ATOMS
PRODUCES f'' FINE STRUCTURE

DAFS

$(\vec{p} \cdot \vec{A})^2$



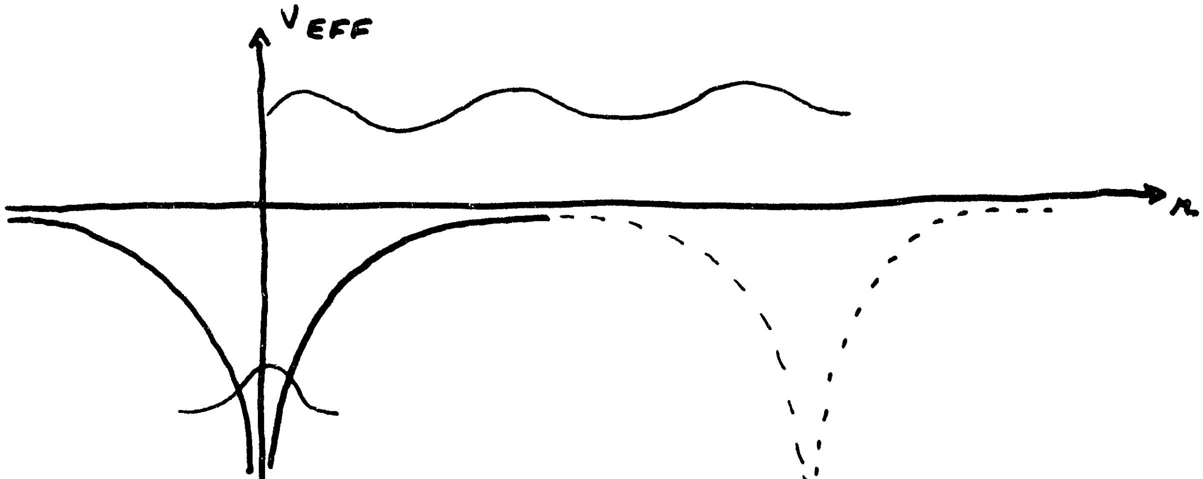
VIRTUAL ELECTRON-HOLE PAIR

VIRTUAL ELECTRON IN THE INTERMEDIATE STATE
WAVEFUNCTION MODULATED BY THE NEIGHBORING ATOMS
PRODUCES THE f', f'' FINE STRUCTURE

PHOTO ABSORPTION (XAFS)

$$\left| \langle f | \hat{e} \cdot \vec{p} \, e^{i \vec{k} \cdot \vec{r}} | i \rangle \right|^2$$ FERMI'S GOLDEN RULE #2

WAVE FUNCTIONS



ELASTIC SCATTERING (DAFS) $\Delta f(\vec{k}_1, \vec{k}_2, \hat{e}_1, \hat{e}_2, E)$

$$\left| \sum_m \frac{\langle i | \hat{e}_2 \cdot \vec{p} \, e^{-i \vec{k}_2 \cdot \vec{r}} | m \rangle \langle m | \hat{e}_1 \cdot \vec{p} \, e^{+i \vec{k}_1 \cdot \vec{r}} | i \rangle}{E_m - E_i - \hbar\omega - i\alpha} \right|^2$$

FERMI'S GOLDEN RULE #1 !

SEPARATE f INTO: FORM FACTOR $\vec{Q}$

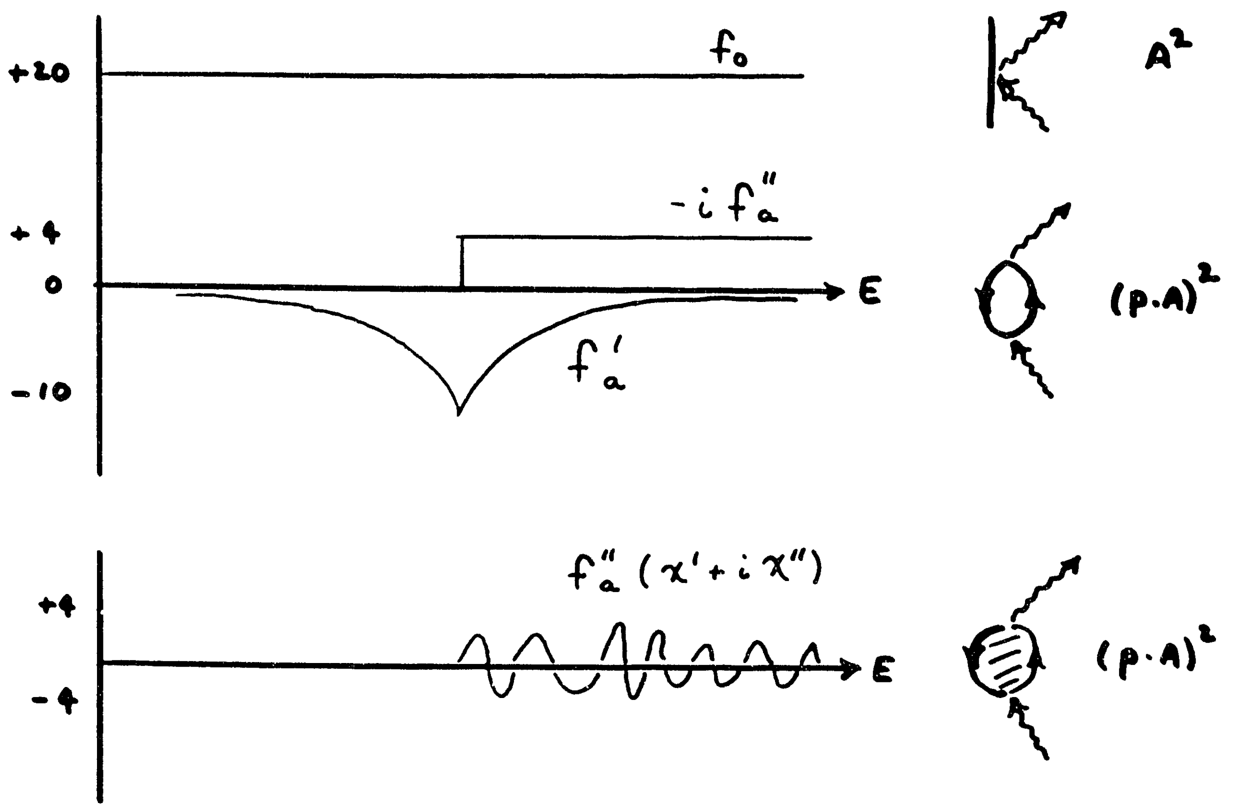
SMOOTH ATOMIC E

DAFS OSCILLATIONS E

$$f = f_0(\vec{Q})$$ THOMSON

$$+ \left[f_a'(E) + i f_a''(E) \right]$$ SMOOTH ATOMIC

$$+ f_a''(E) \left[\chi'(E) + i \chi''(E) \right]$$ DAFS OSCILLATIONS



⇒ TENSOR: 1/4 – 1/2 ELECTRON

DAFS $\chi(E) = \chi'(E) + i\chi''(E) \Rightarrow \chi(K)$

PHOTOELECTRON WAVENUMBER $K = \sqrt{\frac{2m(E-E_0)}{\hbar^2}}$

$$\chi(K) \sim \sum_j N_j \frac{t_j(2K)}{K^2 r_j^2} e^{-2K^2\sigma_j^2} e^{-2r_j/\lambda} e^{-i(2Kr_j + \delta_j(K))}$$

$$\Rightarrow \boxed{-\cos(2Kr_j + \delta_j(K)) + i\sin(2Kr_j + \delta_j(K))}$$

XAFS $\chi_a(K)$

$\chi_a(K) = \operatorname{Im} \chi(K) = \chi''(K)$

$$\Rightarrow \boxed{+\sin(2Kr_j + \delta_j(K))}$$

DAFS AND XAFS CONTAIN THE SAME STRUCTURAL INFORMATION

DAFS: χ' AND χ'' CONTRIBUTIONS

XAFS: χ'' CONTRIBUTION

FOUR SYSTEMS:

1) THIN EPITAXIAL COPPER FILMS
   SIMPLE STANDARD

2) In Ga As MULTILAYERS
   SPATIAL SELECTIVITY

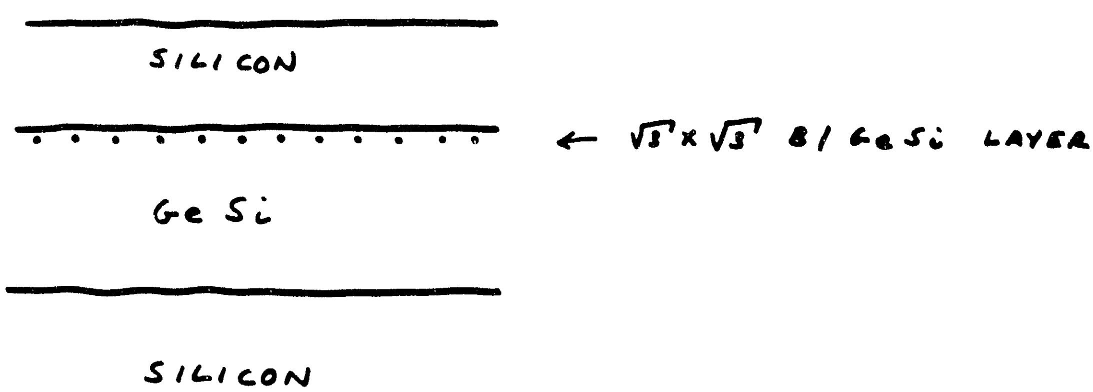
3) 123 SUPERCONDUCTOR THIN FILMS
   SITE SELECTIVITY & VALENCE SENSITIVITY

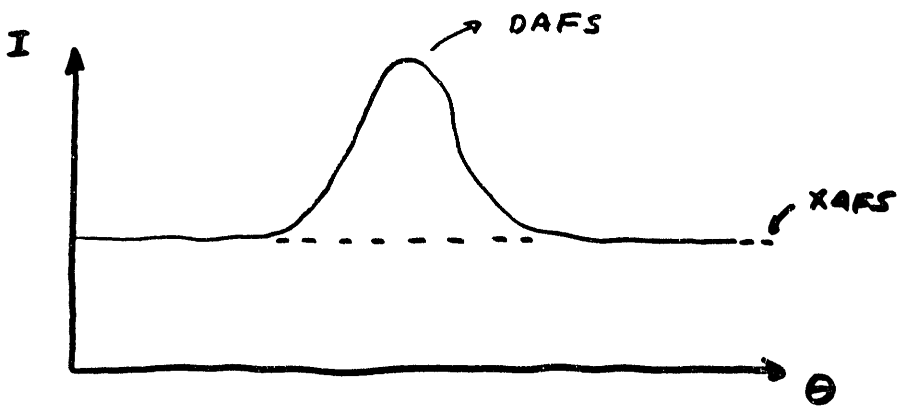
4) Si/B/Ge Si HETEROSTRUCTURE
   MONOLAYER SENSITIVITY

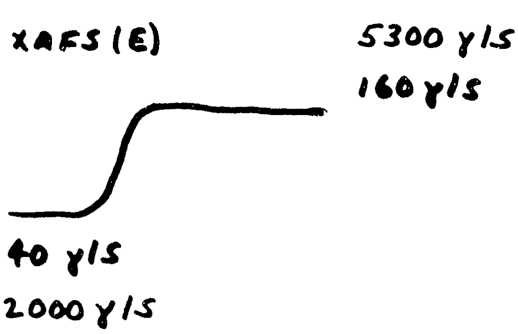
BURIED MONOLAYER DAFS

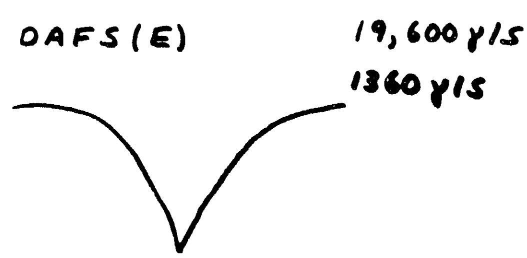
BORON INDUCED $\sqrt{3}$ RECONSTRUCTION OF GeSi

NEC – PF – UW – NIST COLLABORATION

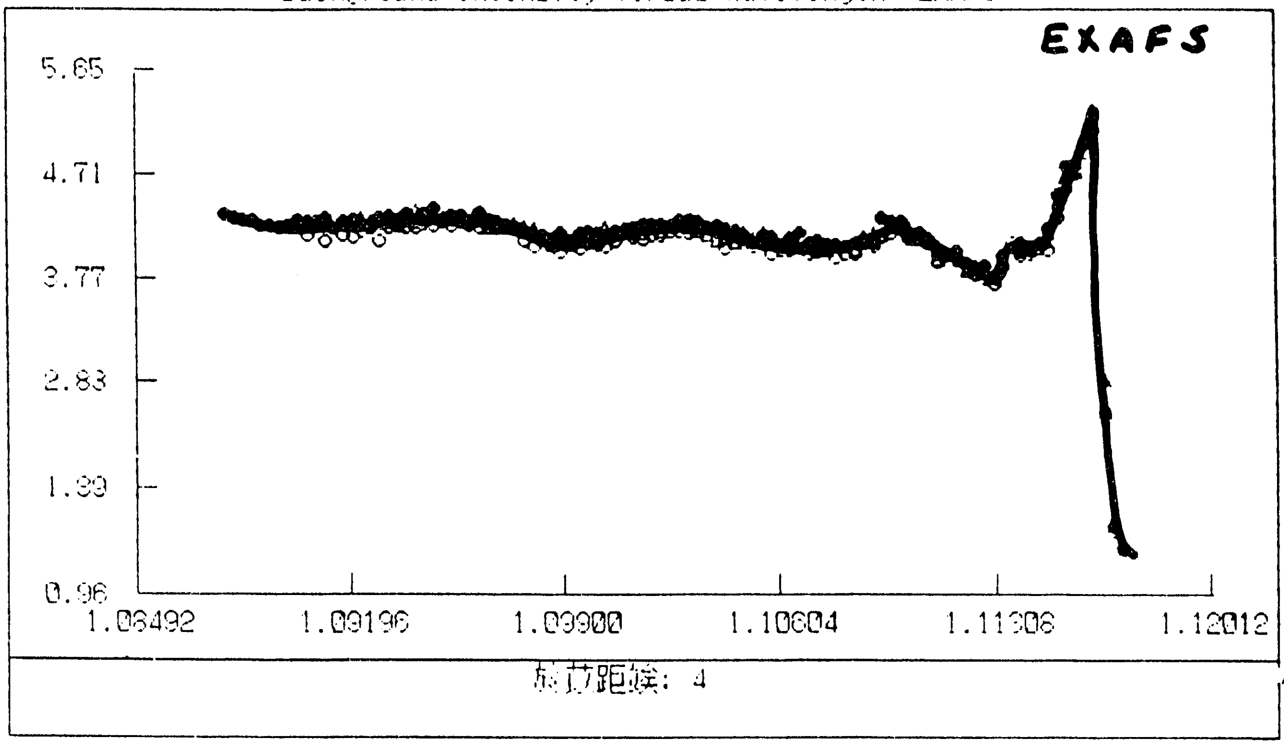




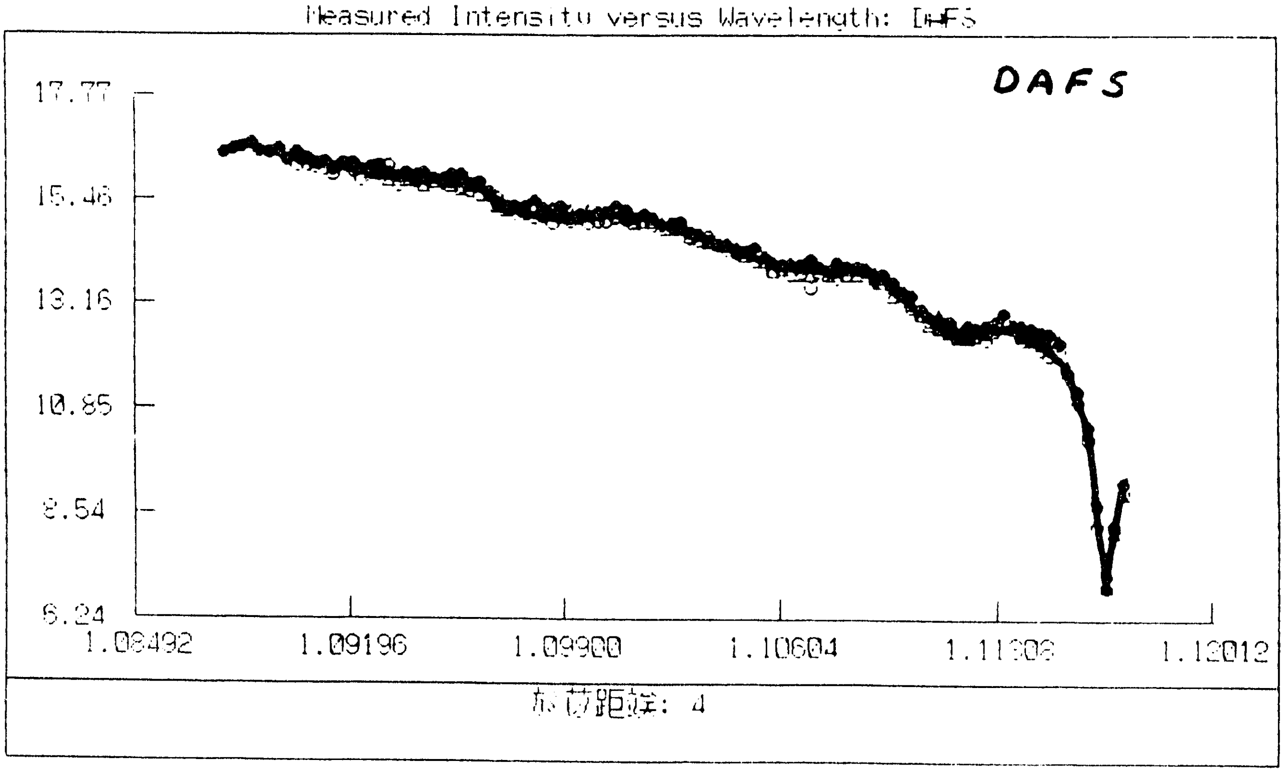




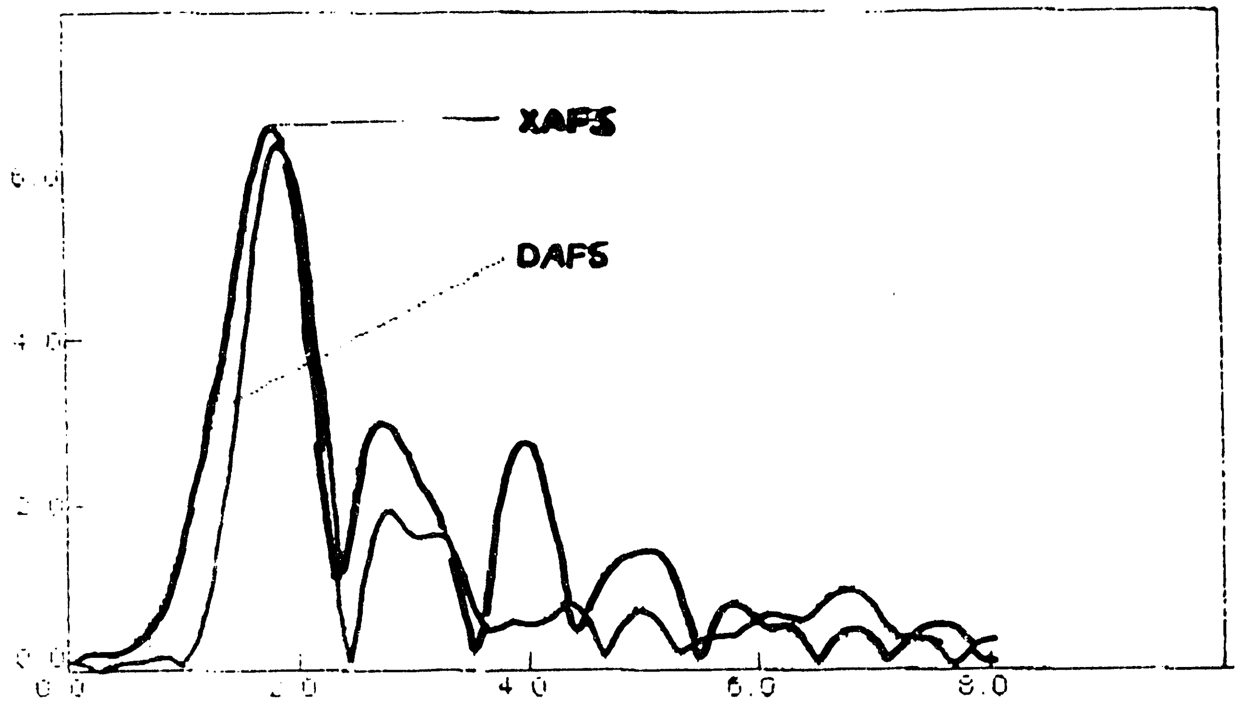
Background Intensity versus Wavelength: EXAFS



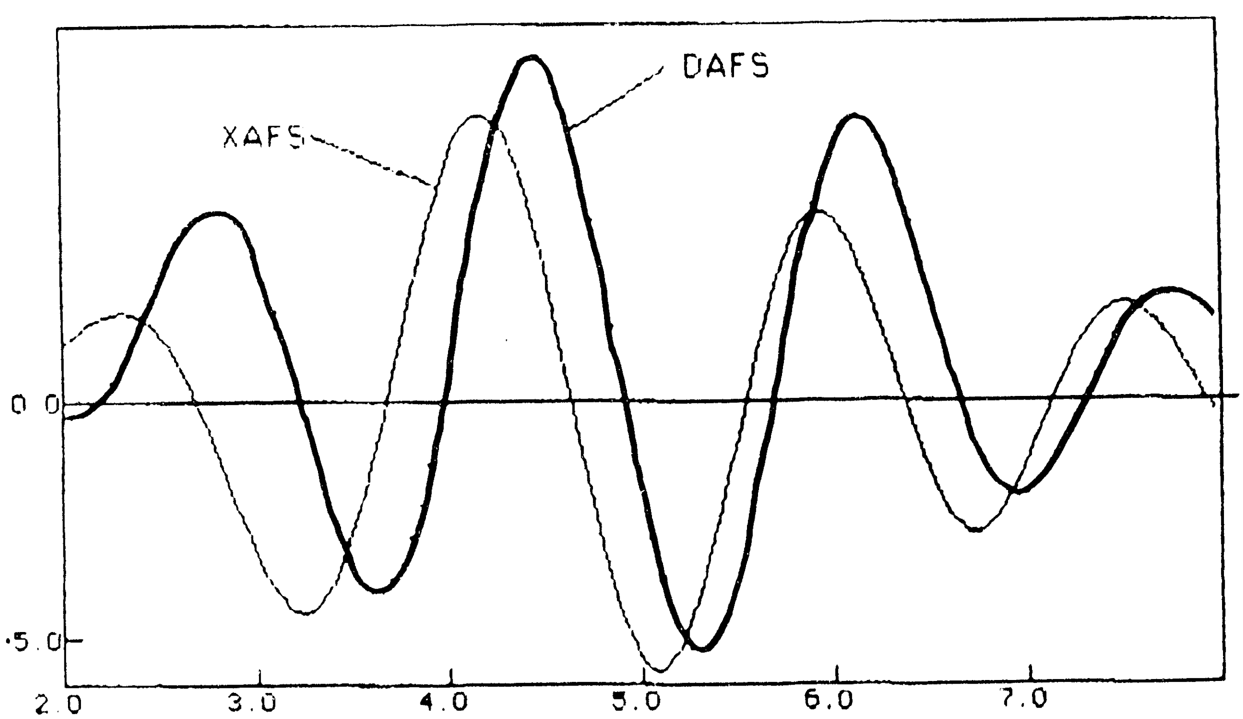
Measured Intensity versus Wavelength: DAFS



GeSi



GeSi first-shell chi data



SITE SENSITIVITY

GOAL: SEPARATE THE LOCAL DAFS ATOMIC STRUCTURAL INFORMATION FOR THE TWO INEQUIVALENT COPPER SITES IN 123 YBaCuO THIN FILMS

VERY WELL KNOWN STRUCTURE
INEQUIVALENT Cu(1) AND Cu(2) SITES

2000 Å THICK $Y_1Ba_2Cu_3O_7$ FILM ON $LaAl_2O_3$

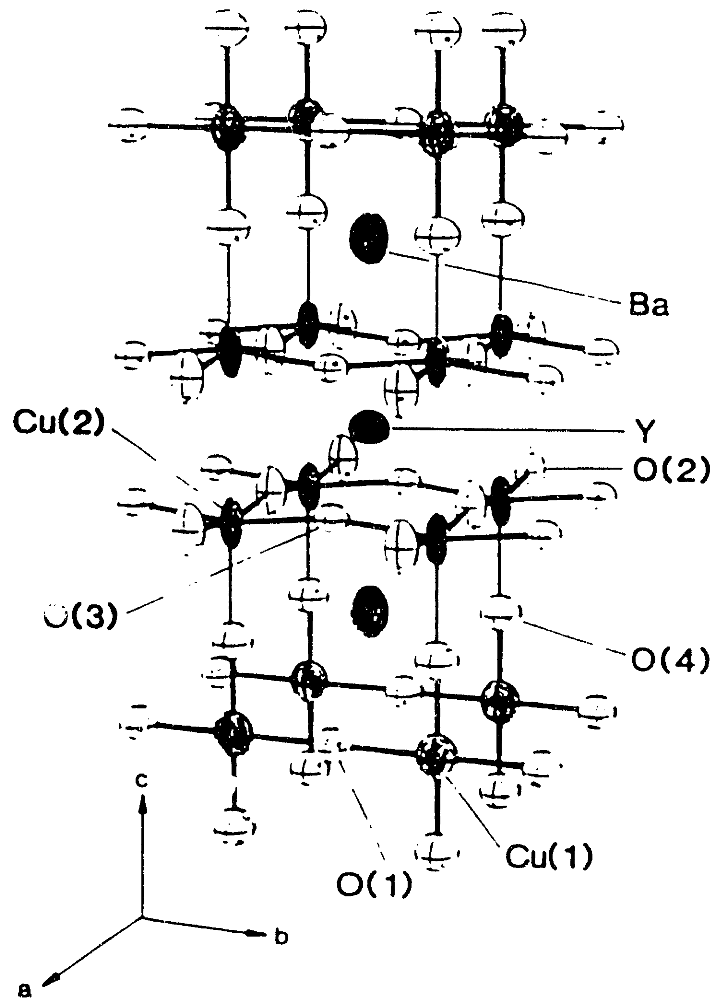
IDEA: EACH BRAGG REFLECTION IS A DIFFERENT LINEAR COMBINATION OF THE TWO COPPER SITE $\tilde{\chi}$'s

Cu (1) $\qquad \tilde{\chi}^1 = \chi_1^1 + i\chi_2^1$

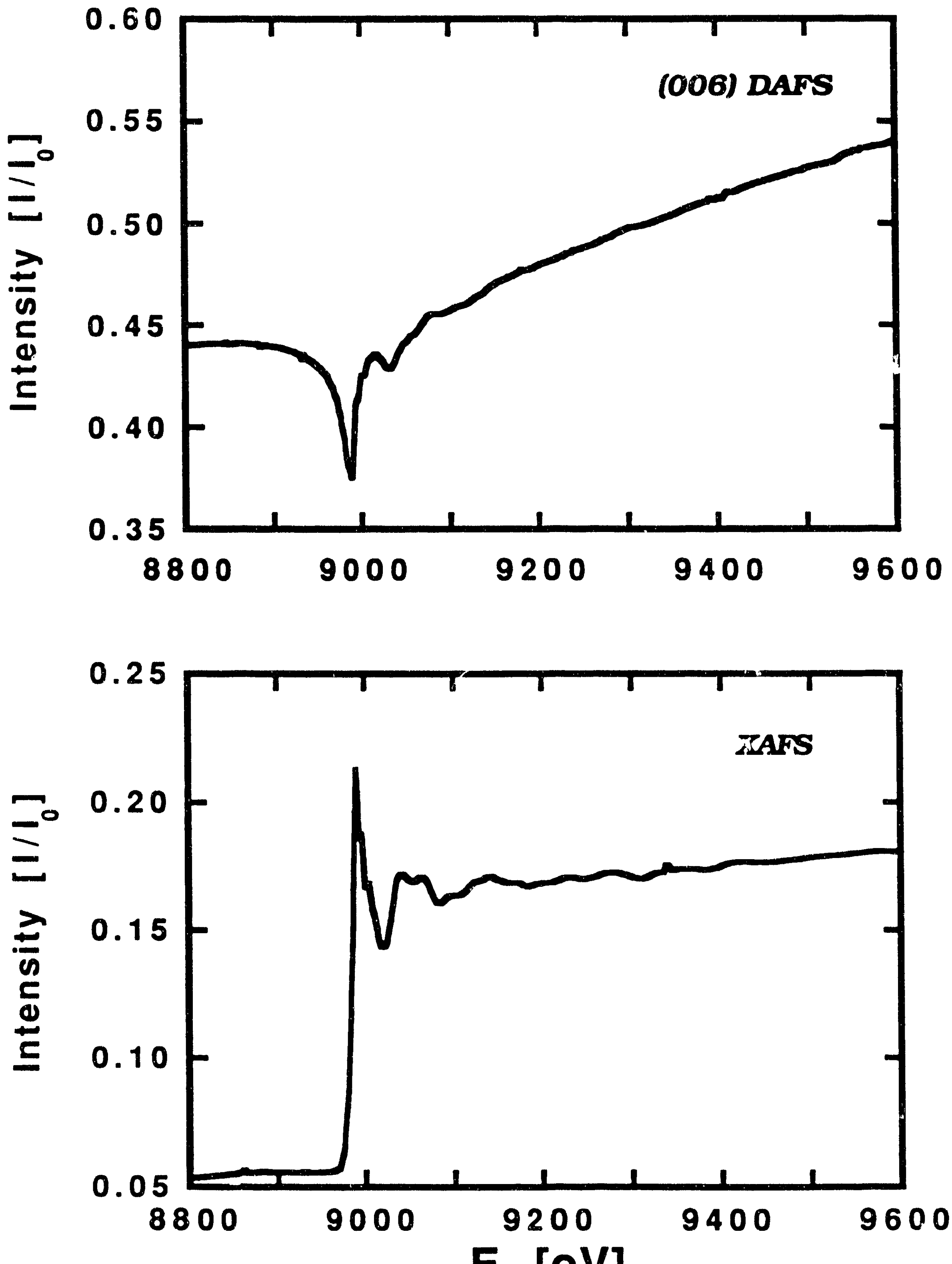
Cu (2) $\qquad \tilde{\chi}^2 = \chi_1^2 + i\chi_2^2$

$$I \sim \text{SMOOTH FCN}(E) + \alpha\left[W_1\chi_1^1 + W_2\chi_1^2\right] + \beta\left[W_1\chi_2^1 + W_2\chi_2^2\right]$$

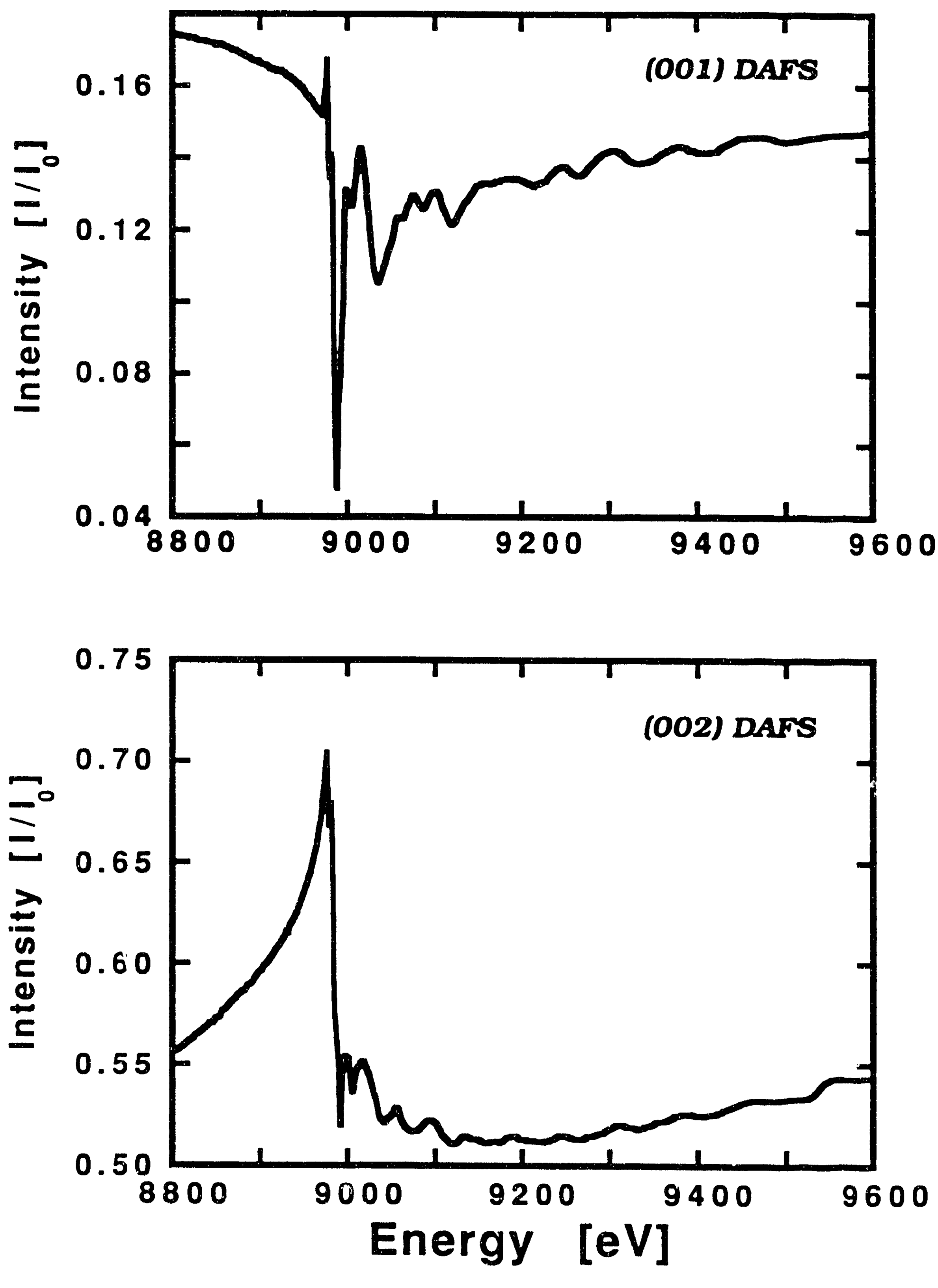
WEIGHTS W_1, W_2 DEPEND ON $\vec{Q}$



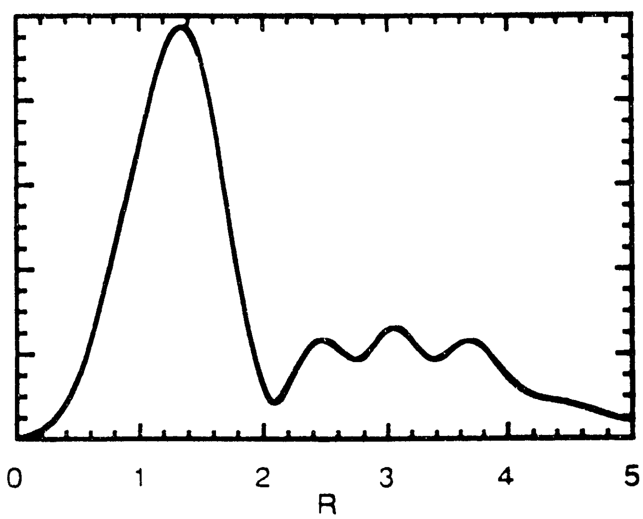
REFLECTION	WEIGHTS CU(1)	WEIGHTS CU(2)
001	1.00	-1.24
003	1.00	1.82
004	1.00	-1.78
006	1.00	1.30
007	1.00	-2.00
XAFS	1.00	2.00



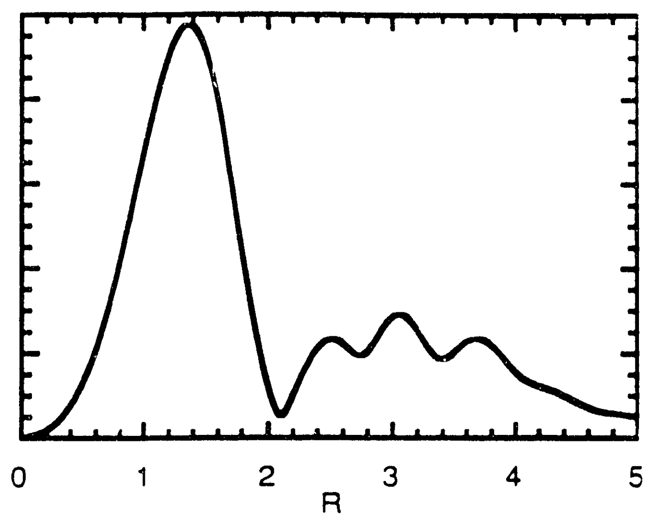
0.60
0.55
0.50
0.45
0.40
0.35
Intensity [I/I0]
(006) DAFS
8800
9000
9200
9400
9600
0.25
0.20
0.15
0.10
0.05
Intensity [I/I0]
XAFS
8800
9000
9200
9400
9600
E [eV]


(001) DAFS
Intensity [I/I0]
0.16
0.12
0.08
0.04
8800
9000
9200
9400
9600
(002) DAFS
Intensity [I/I0]
0.75
0.70
0.65
0.60
0.55
0.50
8800
9000
9200
9400
9600
Energy [eV]

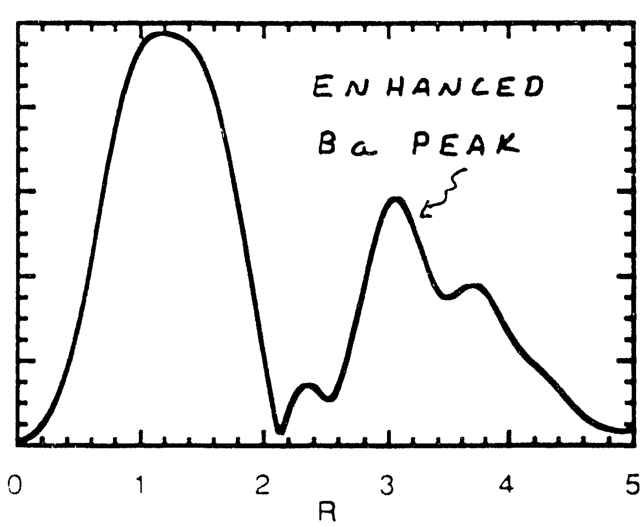
$YBa_2Cu_3O_7$ (003) DAFS



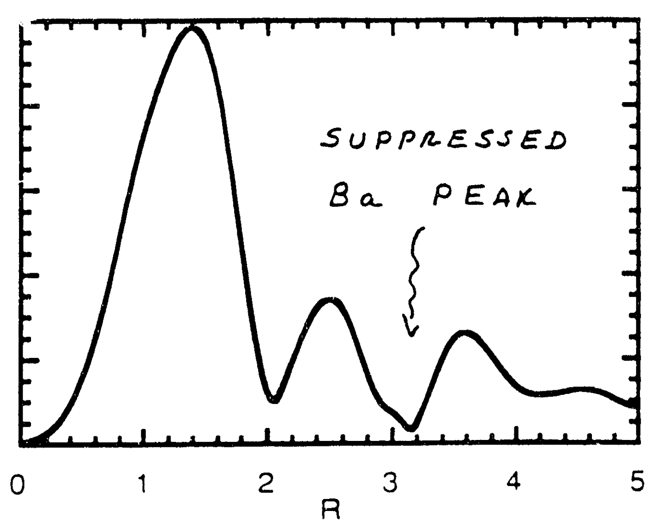
$YBa_2Cu_3O_7$ (006) DAFS



$YBa_2Cu_3O_7$ (005) DAFS



$YBa_2Cu_3O_7$ (007) DAFS

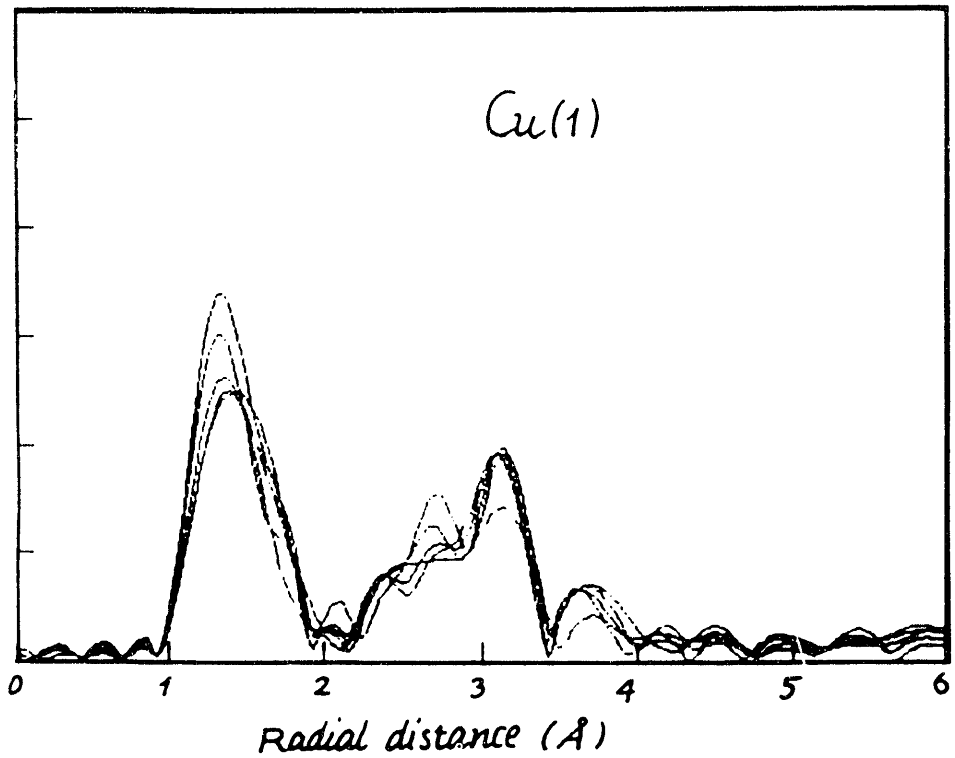


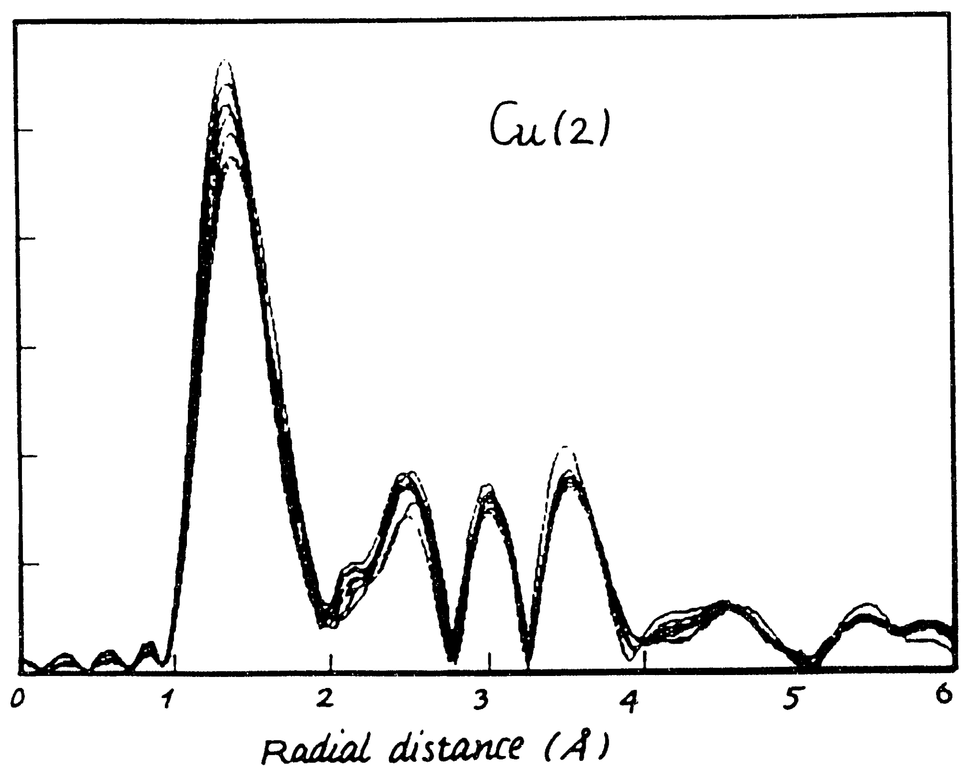
(8) (+1) = + 8

(4) (0.3) = + 1.2

Cu 1 (8) (+1) = + 8

Cu 2 (4) (−2) = − 8


Cu(1)
0
1
2
3
4
5
6
Radial distance (Å)


Cu(2)
0
1
2
3
4
5
6
Radial distance (Å)

DANES

IDEA: USE DAFS CRYSTALLOGRAPHIC SENSITIVITY IN NEAR EDGE REGION TO SEPARATE INEQUIVALENT SITES.

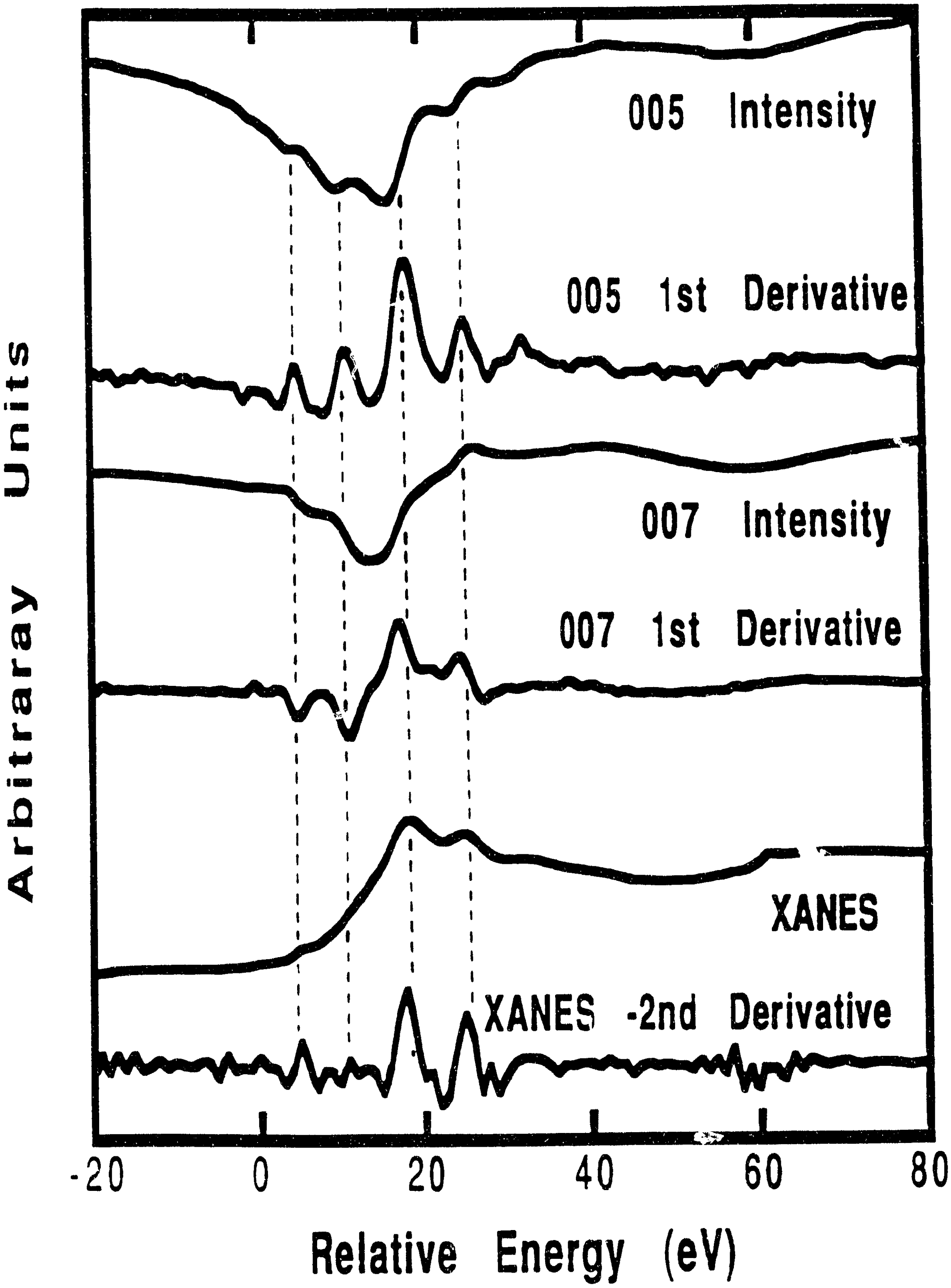
DIFFRACTION → XANES

ADDS CRYSTALLOGRAPHIC SITE SELECTIVITY

DANES → DIFFRACTION

ADDS VALENCE AND ORBITAL SENSITIVITY

YBCuO DANES and XANES



RÖHLER ET. AL. PHYSICA C 191, 57 (1992)

5eV 1) Cu(1) and Cu(2) $1s \rightarrow 4p^{*}\pi$ SHAKEDOWN CHARGE TRANSFER SATTELLITE

OR

FINAL STATE DELOCALIZED OVER LARGE CLUSTE

12eV 2) Cu(2) $1s \rightarrow 4p\pi_z$ OUT-OF-PLANE "SAFELY ASSIGNED!"

17eV 3) Cu(1) $1s \rightarrow 4p_y\sigma$

OR

Cu(2) $1s \rightarrow 4p_{xy}\sigma$

25eV 4) Cu $3d^8$

OR

Cu - O INDICATING Cu-Y ANTISITE DISORDER

OR

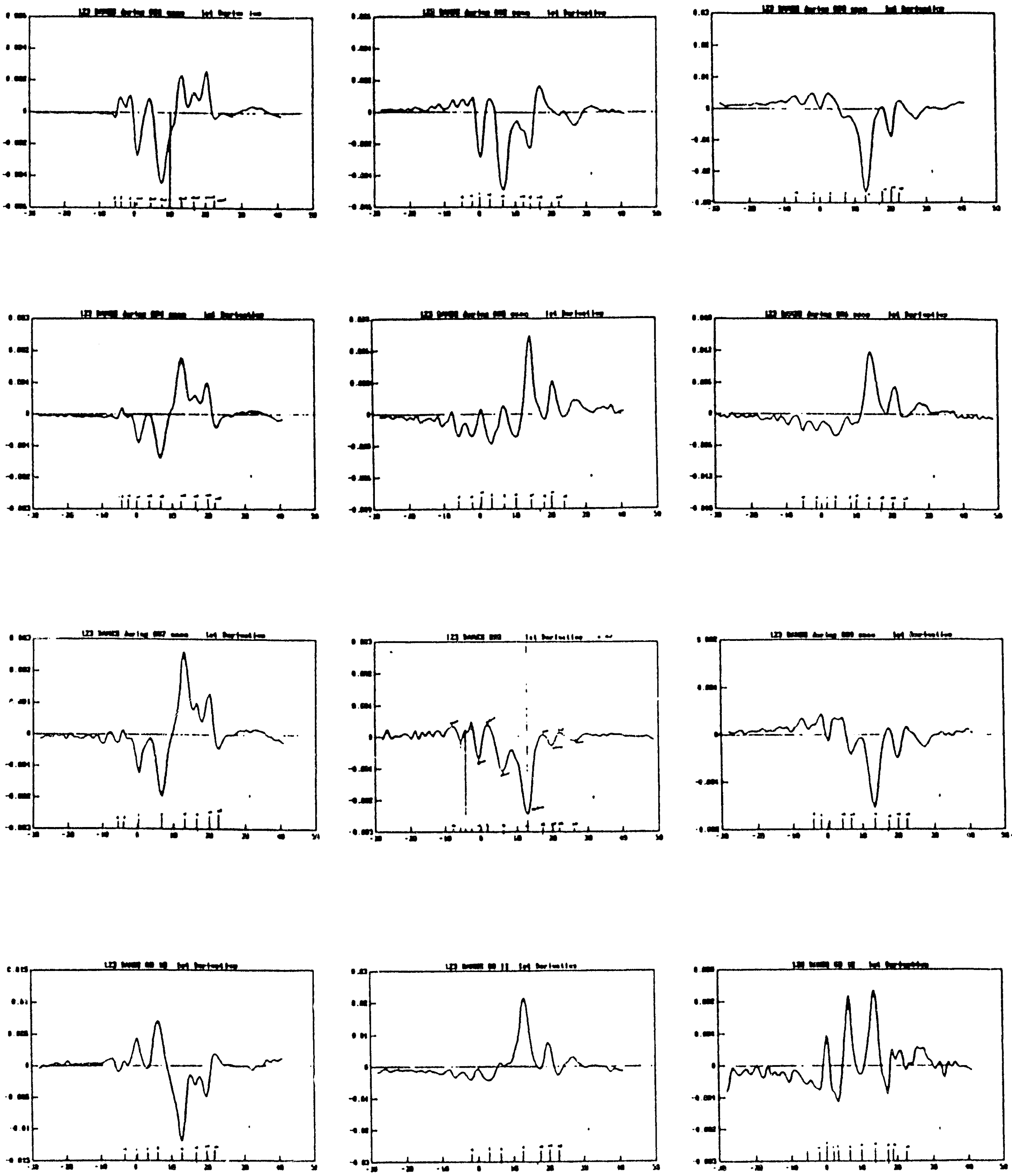
[Cu(1) O_m] CLUSTER EXCITATION WITH $m > 6$

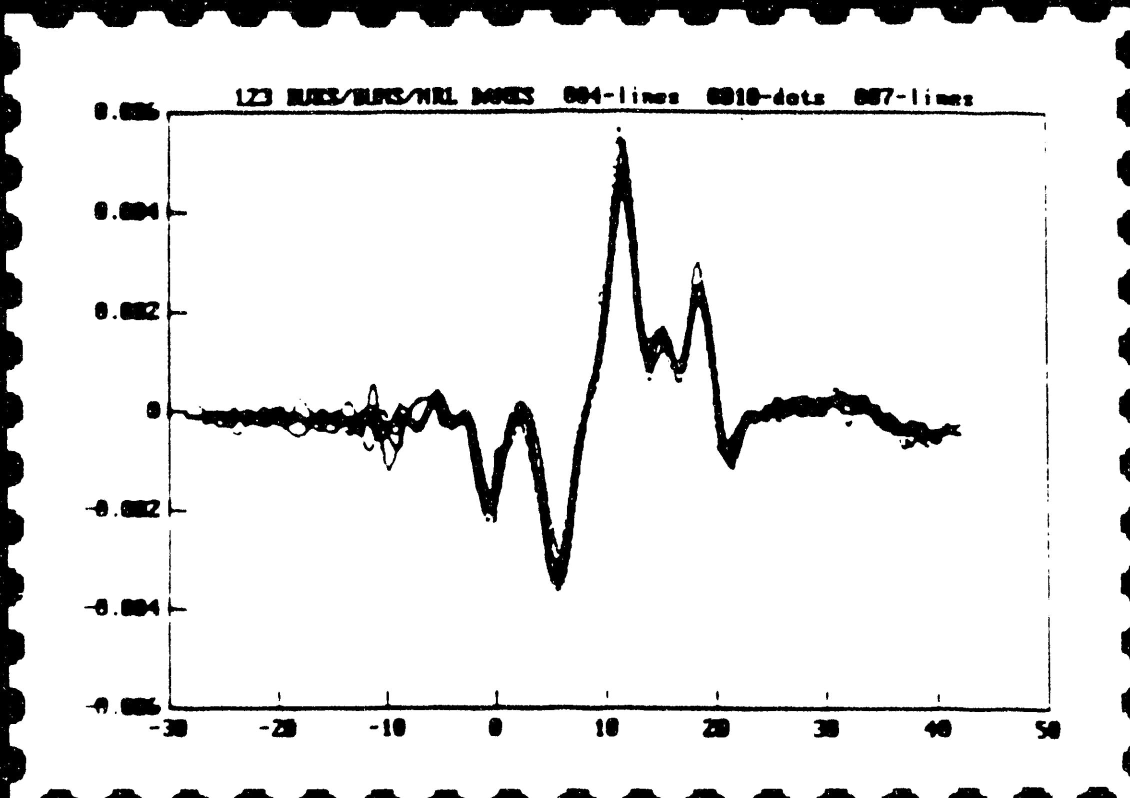
" THERE IS PHYSICS,

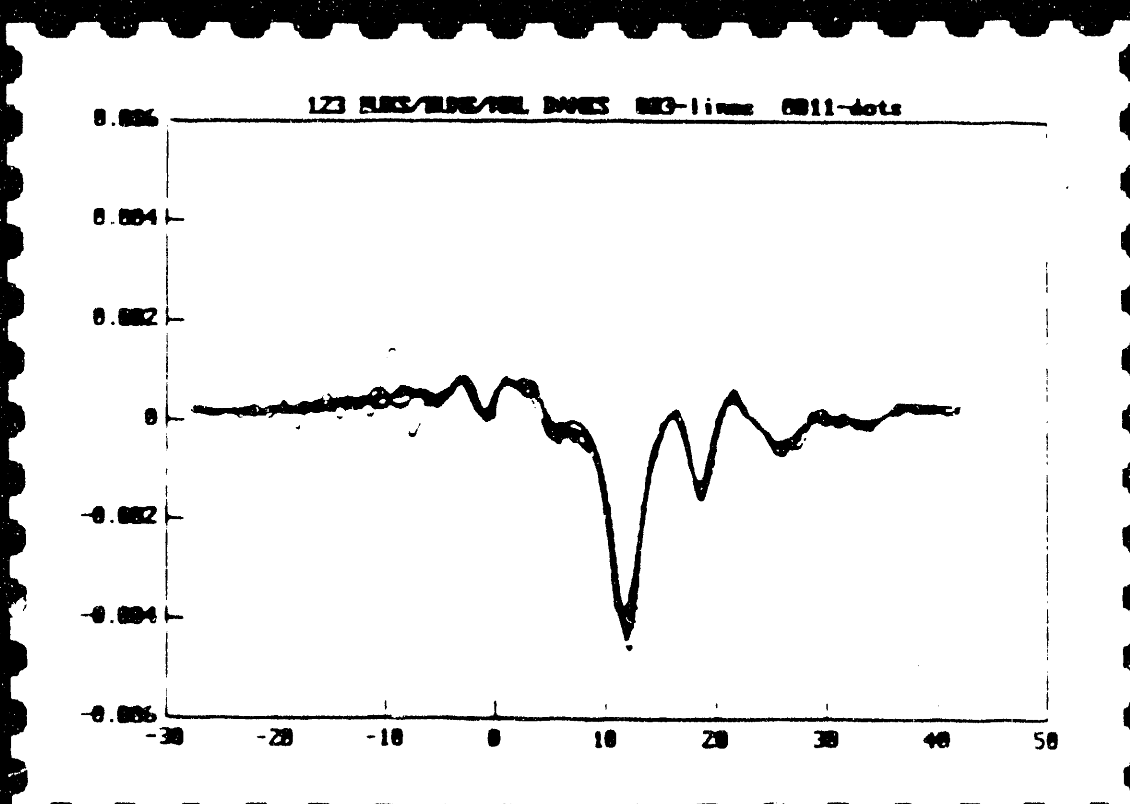
AND THEN THERE IS STAMP

COLLECTING "

E. RUTHERFORD




0
-30
-20
-10
0
10
20
30
40
50


0
-30
-20
-10
0
10
20
30
40
50

SUMMARY

DAFS PROVIDES:

1) SPATIAL SELECTIVITY VIA $\vec{Q}$

WHENEVER $\{\alpha_1(\vec{r})\} \neq \{\alpha_2(\vec{r})\}$

2) SITE SELECTIVITY VIA INTENSITIES FOR INEQUIVALENT SITES

3) VALENCE SELECTIVITY VIA DANES FOR MIXED VALENCE IN EQUIVALENT SITES

FUTURE ?

	PDAFS, P DANES	POLARIZATION
	McDAFS, McDANES	MAGNETIC CIRCULAR
✓	QDAFS, Q DANES	QUADRUPOLE
✓	SWAFS, SWANES	STANDING WAVES
	DDAFS, DDANES	DYNAMICAL
✓	CTR DAFS, CTR DANES	CRYSTAL TRUNCATION ROD

MAD ⟶ CAST

CONVERSATION IN GASLIT HALLS OF THE 1851 LONDON EXHIBITION:

VISITOR: "WHAT POSSIBLE USE CAN ARISE FROM YOUR EXPERIMENTS ON ELECTRICITY?"

FARADAY: "OF WHAT USE IS A NEW BORN BABY?"

PHOTON ECOLOGY

USE ALL THE DEGREES OF FREEDOM/ QUANTUM NUMBERS OF YOUR PHOTONS!

1) MOMENTUM

2) ENERGY

3) SPIN / POLARIZATION

Coherent X-ray Optics: Soft X-ray Microscopes and Making Things Harder

Chris Jacobsen, Department of Physics, SUNY Stony Brook

ABSTRACT

The advent of undulator sources on low emittance storage rings is enabling several groups to make new advances in x-ray optics. Using a soft x-ray undulator at the NSLS x-ray ring, we have developed a scanning transmission microscope that is able to image <50 nm structures in wet, thick biological specimens; other additional imaging modalities are also being developed. In addition, we are also developing holographic approaches to microscopy and to the design of diffractive masks for projection x-ray lithography. Scaling of these experiments to shorter wavelengths will be discussed, and some new opportunities that may be afforded by the APS will be considered.

X-ray microscopy at X-1

Development of new modalities

- XANES from sub-0.1 μm spot
- X-ray luminescence
- Zernicke and differential phase contrast
- Selected area diffraction
- Stereo and tomographic imaging
- Holographic microscopy

Applications

- Radiation damage studies
- Cellular anatomy and ultrastructure
- Biochemical mapping? (XANES and luminescence)
- Elemental analysis (mostly Ca)
- Polymer properties

What APS would do

- Microanalysis with high spatial resolution (P, S, Ca)
- Microdiffraction (optimum at ~ 1 keV)
- Thicker water layers
- Thicker samples
- Micro-XANES on $Z > 8$ K-edges

What is needed

- Modest to high coherence at 0.5–5 keV (both spatial and temporal)
- Beam/beamline stability to $\ll \sigma$
- Micropositioning/scanning system with < 30 nm resolution, noise
- Remote sample control capabilities (wet cell pumps, etc)
- Support facilities including wet lab, optical microscopes.

The X-1A crew

Stony Brook Physics: Henry Chapman, Hasan Imam, Chris Jacobsen, Janos Kirz, Cheng-Hao Ko, Steve Lindaas, Shawn Williams, Sue Wirick, Xiaodong Zhang

Lawrence Berkeley Laboratory: Erik Anderson, David Attwood, Kaarin Goncz, Malcolm Howells, Mario Moronne, Max Wei

IBM T. J. Watson Research Center (Yorktown Heights): Dieter Kern, David Sayre (ret.)

National Synchrotron Light Source (Brookhaven): Steve Hulbert, Erik Johnson

North Carolina State University: Harald Ade

Advanced Photon Source (Argonne): Ian McNulty

UC San Francisco: Stephen Rothman

Especially frequent visitors:

Livermore: James Trebes

King's College, London: Christopher Buckley, Ronald Burge, Graeme Morrison

CalTech: Jerry Pine

Thanks! to DoE OHER
NSF Bio Instrument Dev,
Pres. Faculty Fellow

Why soft x-rays?

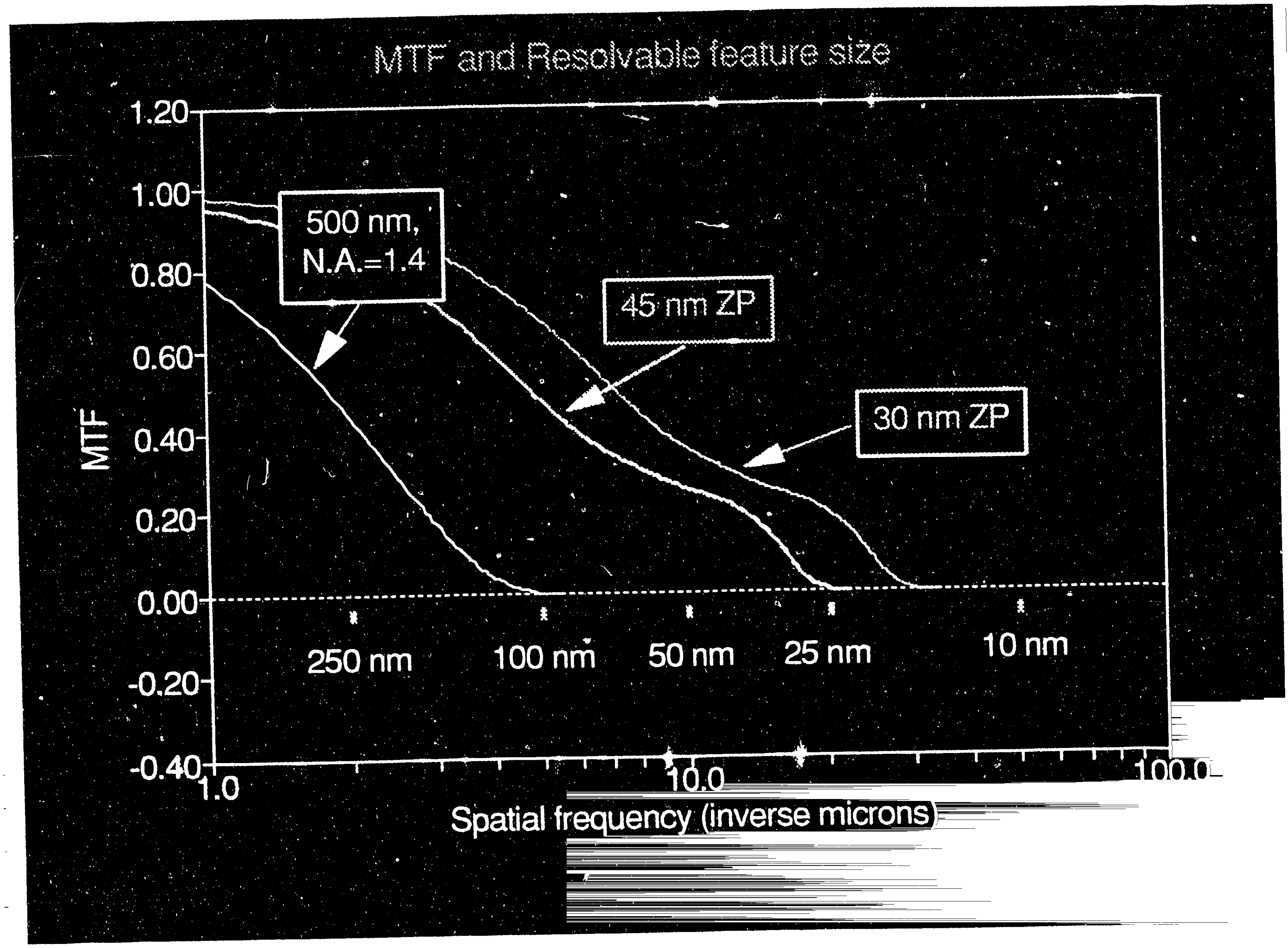
- Short λ: better resolution than optical microscope
- Wet specimens:

$$2.3nm \leq \lambda \leq 4.3nm$$
$$\text{(Oxygen } K) \qquad \text{(Carbon } K)$$

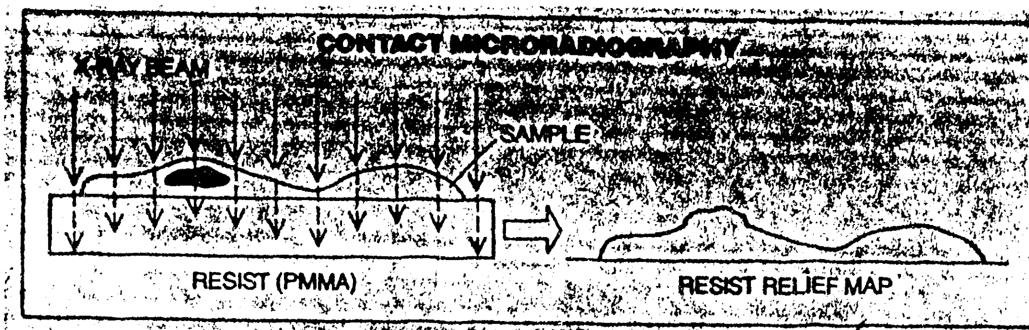
- Thicker specimens than electron microscope (no multiple scattering)
- Lower dose than electron microscope (although dose is still in the megarad range)
- Some elemental mapping capabilities

These basic advantages have been known for ~40 years. Until recently, however, progress has been limited by:

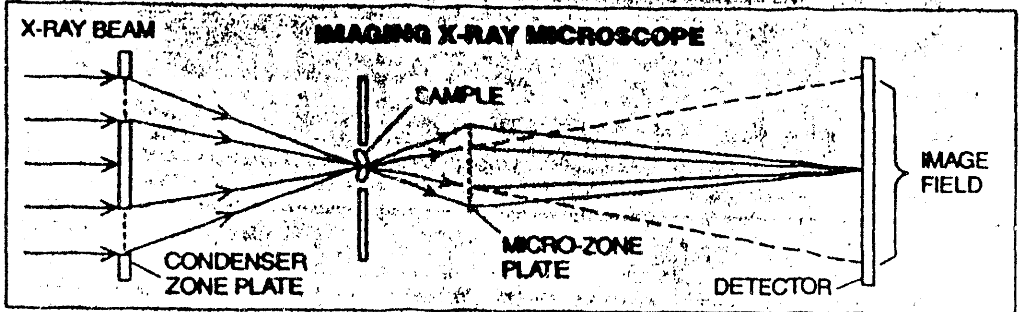
- Lack of bright x-ray sources
- Lack of high resolution optics
- Lack of supporting technologies



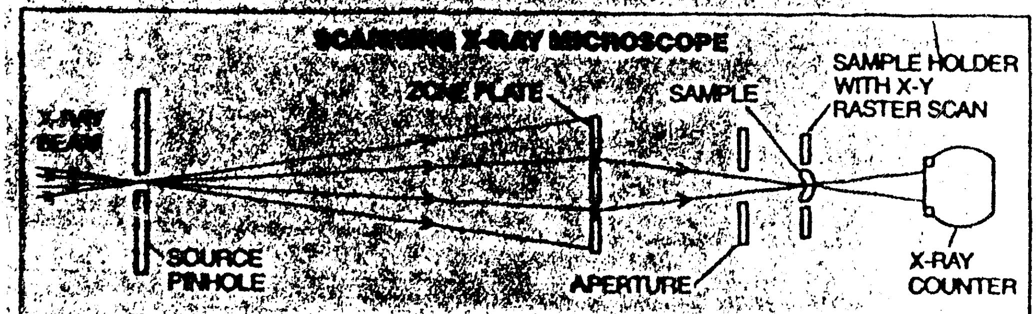
MTF and Resolvable feature size
1.20
1.00
0.80
0.60
0.40
0.20
0.00
-0.20
-0.40
MTF
500 nm,
N.A.=1.4
45 nm ZP
30 nm ZP
250 nm
100 nm
50 nm
25 nm
10 nm
1.0
10.0
100.0
Spatial frequency (inverse microns)



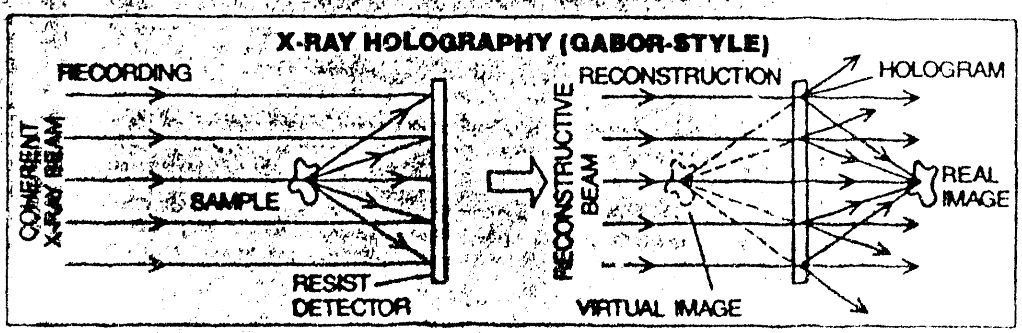
DAMAGE PATTERN in the resist results from the X rays that pass through the sample (*left*). A developer preferentially dissolves the radiation-damaged regions (*right*).



FRESNEL ZONE PLATES serve as condenser and objective X-ray lenses. The former focus a beam on a sample; the latter magnify images of the sample on a detector.



FOCUSED X-RAY BEAM scans back and forth, top to bottom across the sample; the rays that penetrate at each point are measured using a proportional X-ray counter.

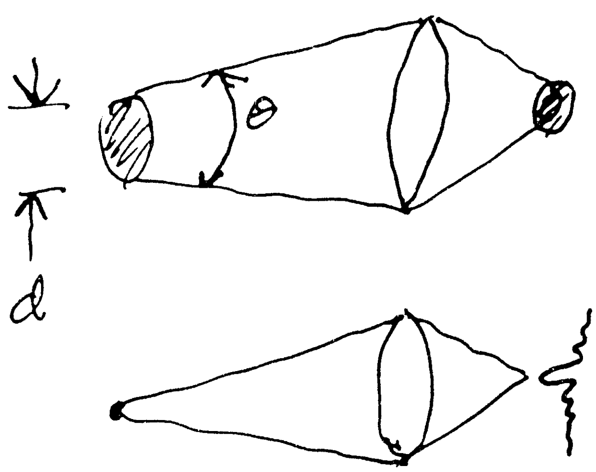


INTERFERING incident and scattered X-ray beams record a hologram in a sheet of resist (*left*). The image is reconstructed (*right*) either by illuminating the hologram with laser light or by digitizing the hologram and performing a computation on it.

● ZBC 915-4070

Spatial coherence in scanning microscopes

$$\#\text{ modes} \sim \frac{(d\cdot\theta)_H}{\lambda} \cdot \frac{(d\cdot\theta)_V}{\lambda}$$



Geometrical image of source

Diffraction-limited image

Partial coherence in scanning microscopes

Scanning transmission microscopes with large detectors give incoherent brightfield images. However, resolution is limited by the coherence of the light illuminating the probe-forming objective.

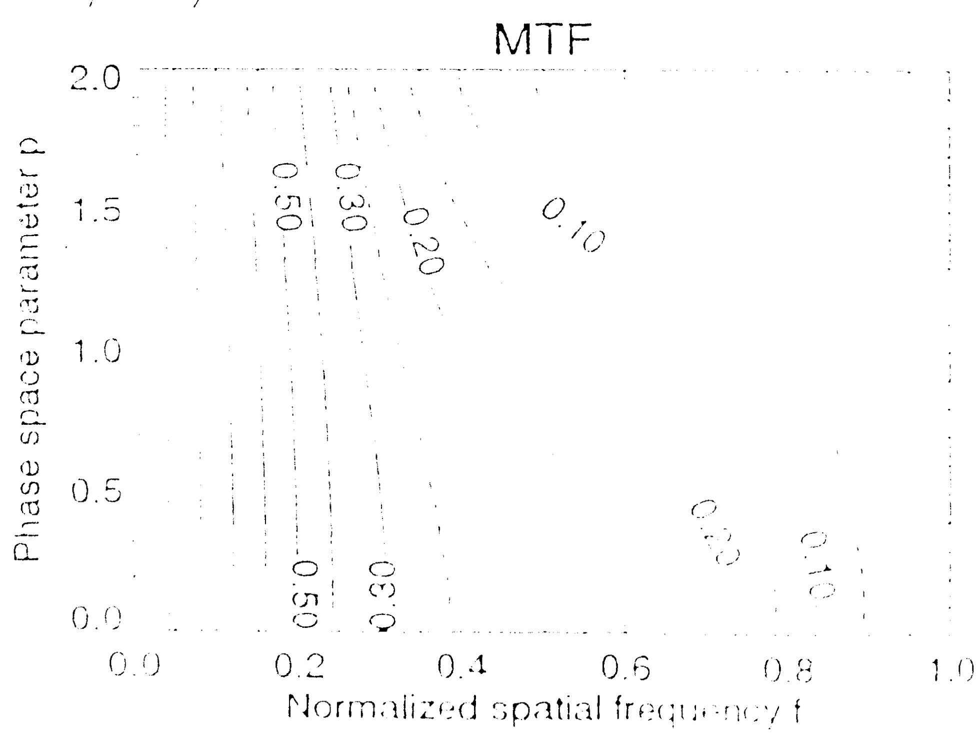
- Focal spot phase space (full width, full angle) with perfect coherence:

$$\begin{aligned} \text{phase space} &= \text{spot width} \cdot \text{beam angle} \\ \phi &= \left(2\,\frac{0.61\lambda}{\text{N.A.}}\right)\cdot(2\,\text{N.A.}) \\ &= 2.44\,\lambda \end{aligned}$$

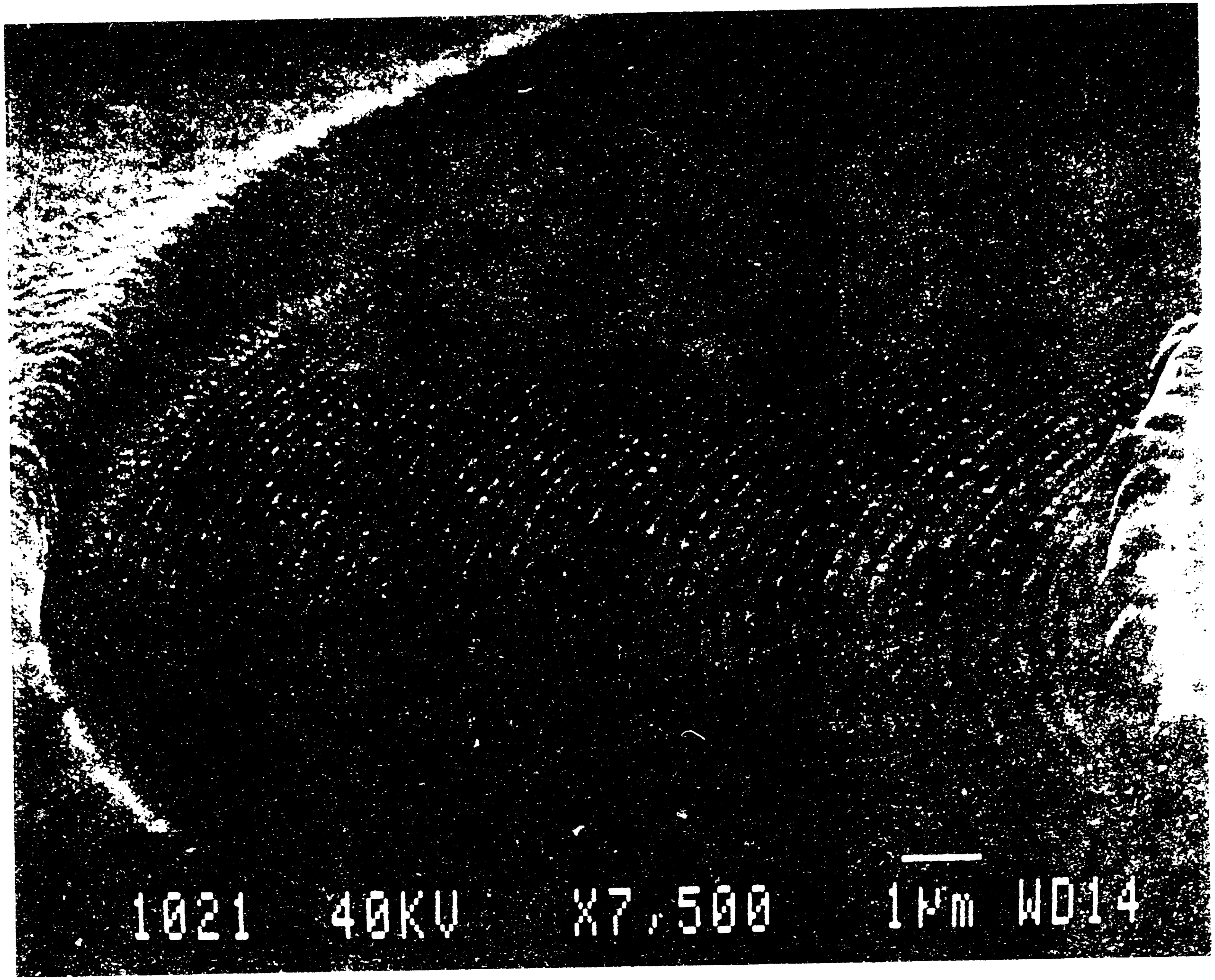
- Characterize illumination phase space as $\phi = p\lambda$, where ϕ is product of source full width and full angle.
- Source phase space parameter of $p = 0.5$–1 gives nearly full resolution.
- Contours of image modulation transfer function MTF for a lens with a half-diameter central stop

  p: phase space parameter (above)

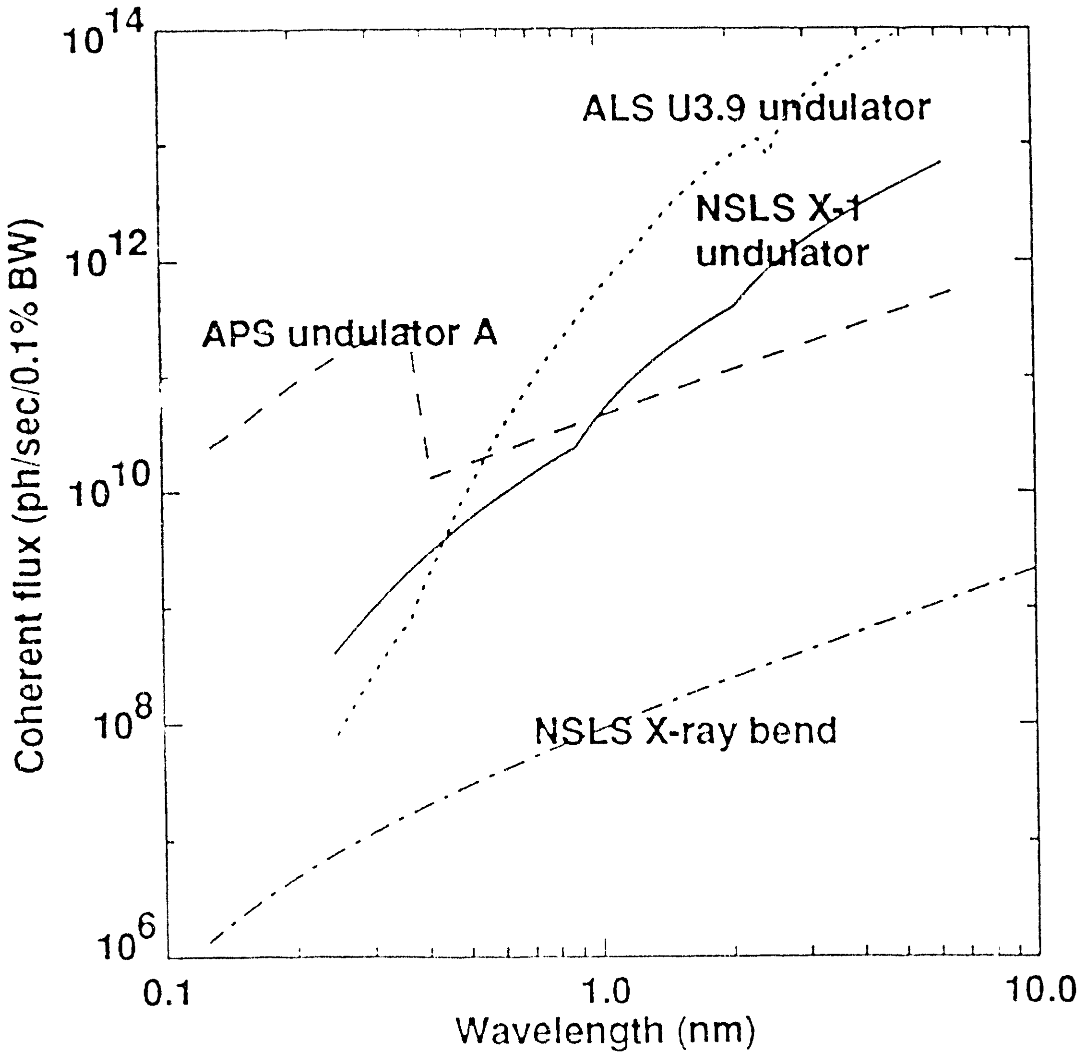
  f: normalized spatial frequency (1.0 corresponds to feature size of $0.25\lambda/\text{N.A.}$)

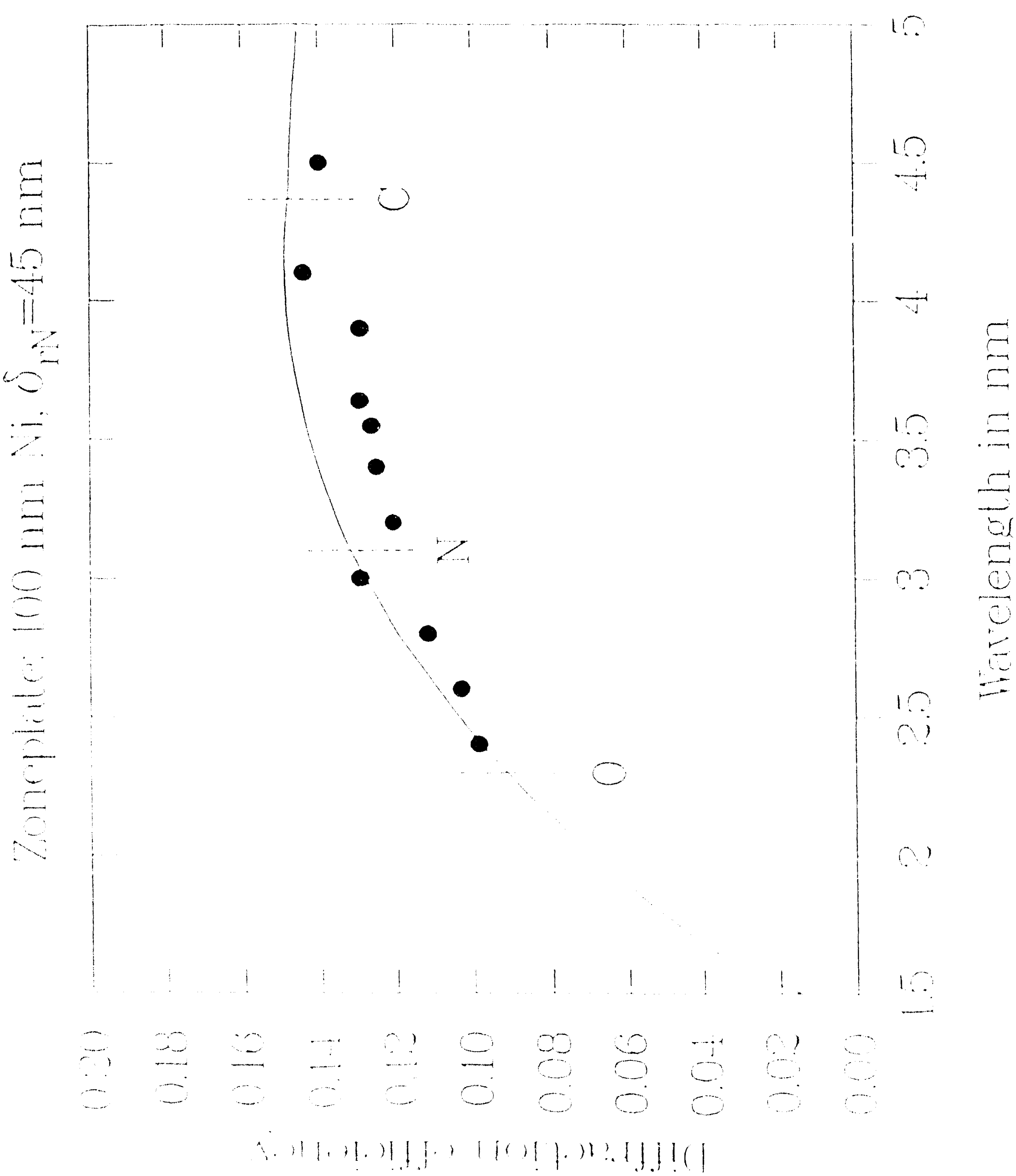


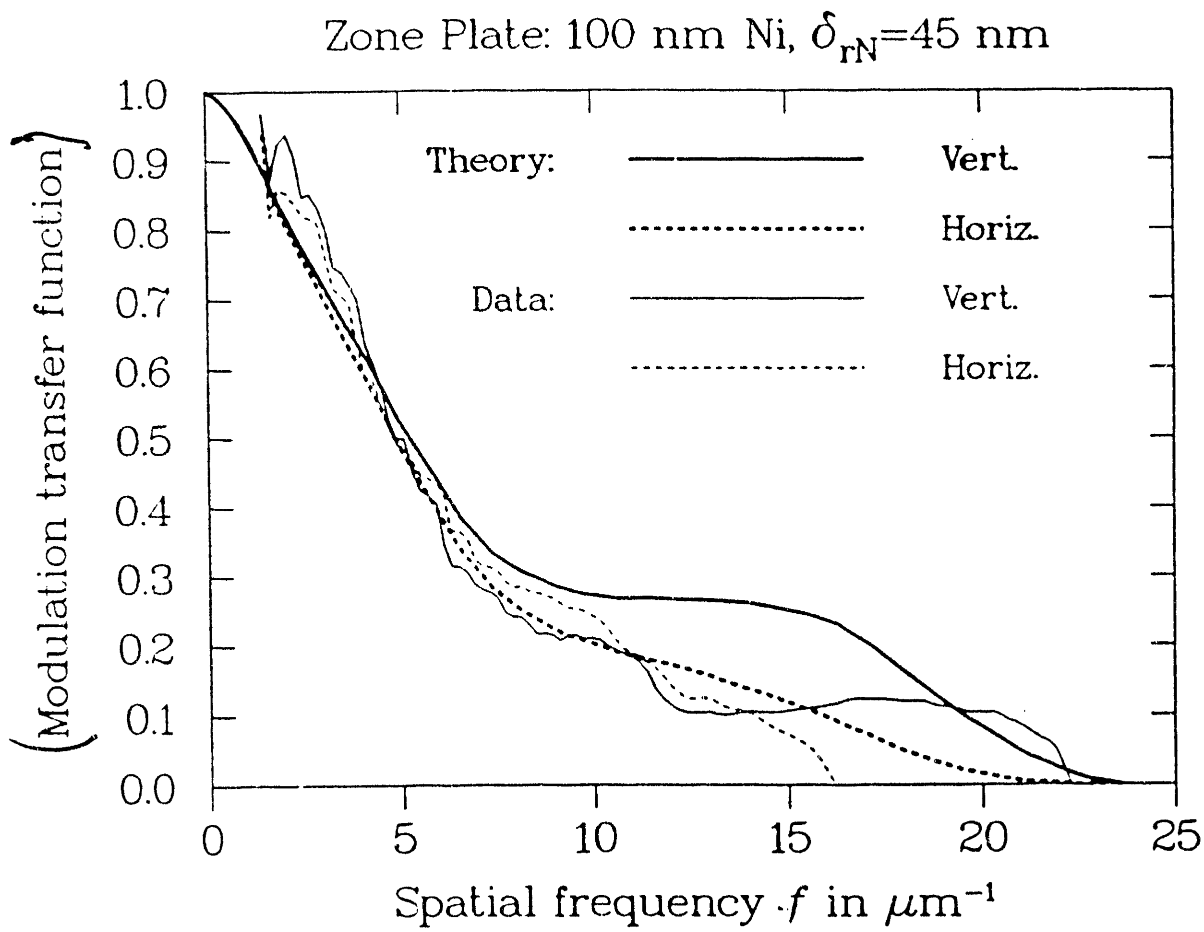
Y. Vladimirsky, Center for X-Ray Optics, LBL / IBM 3/1986



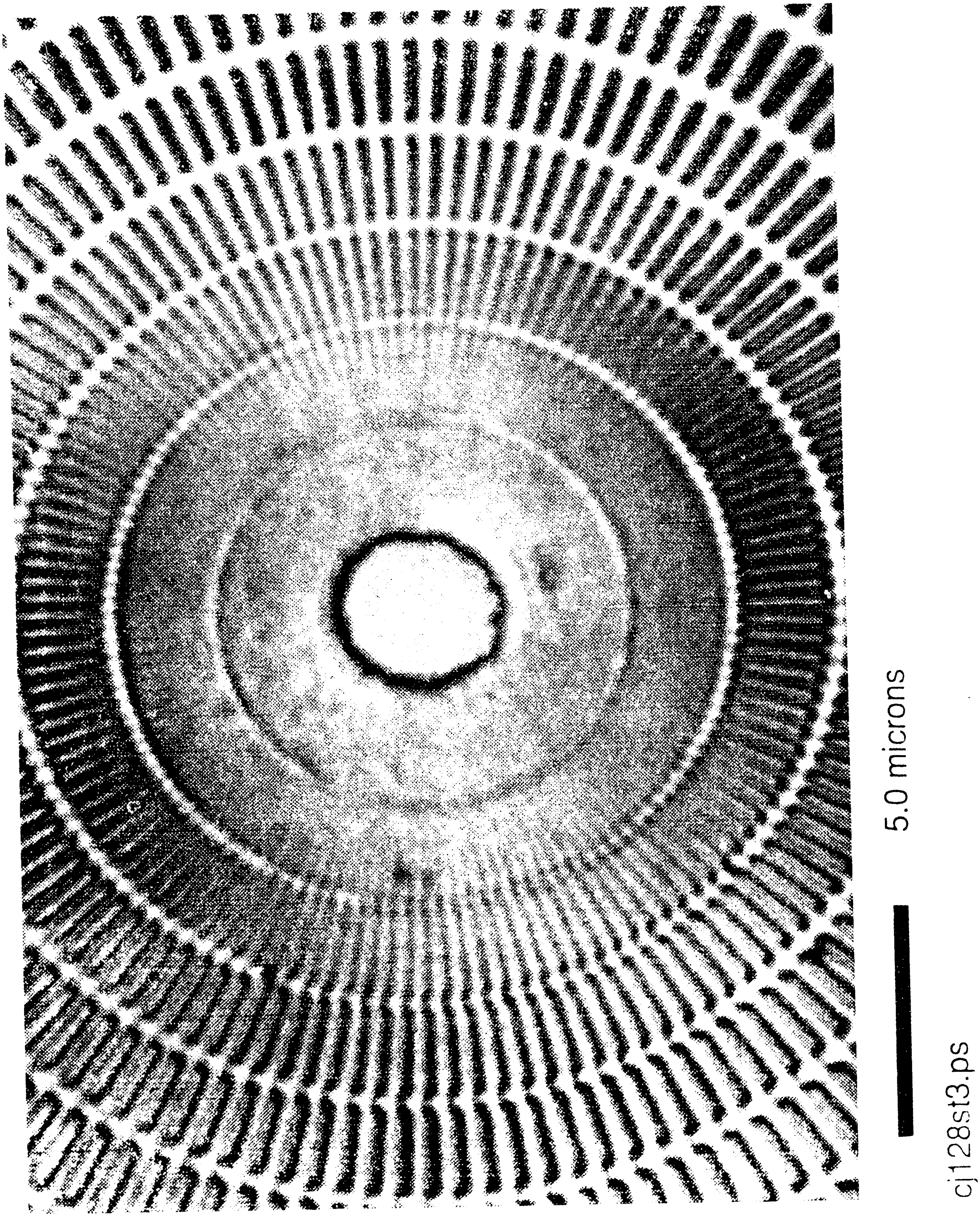
XBB 863-1722 ≥0.2μm period, ~0.13μm thin

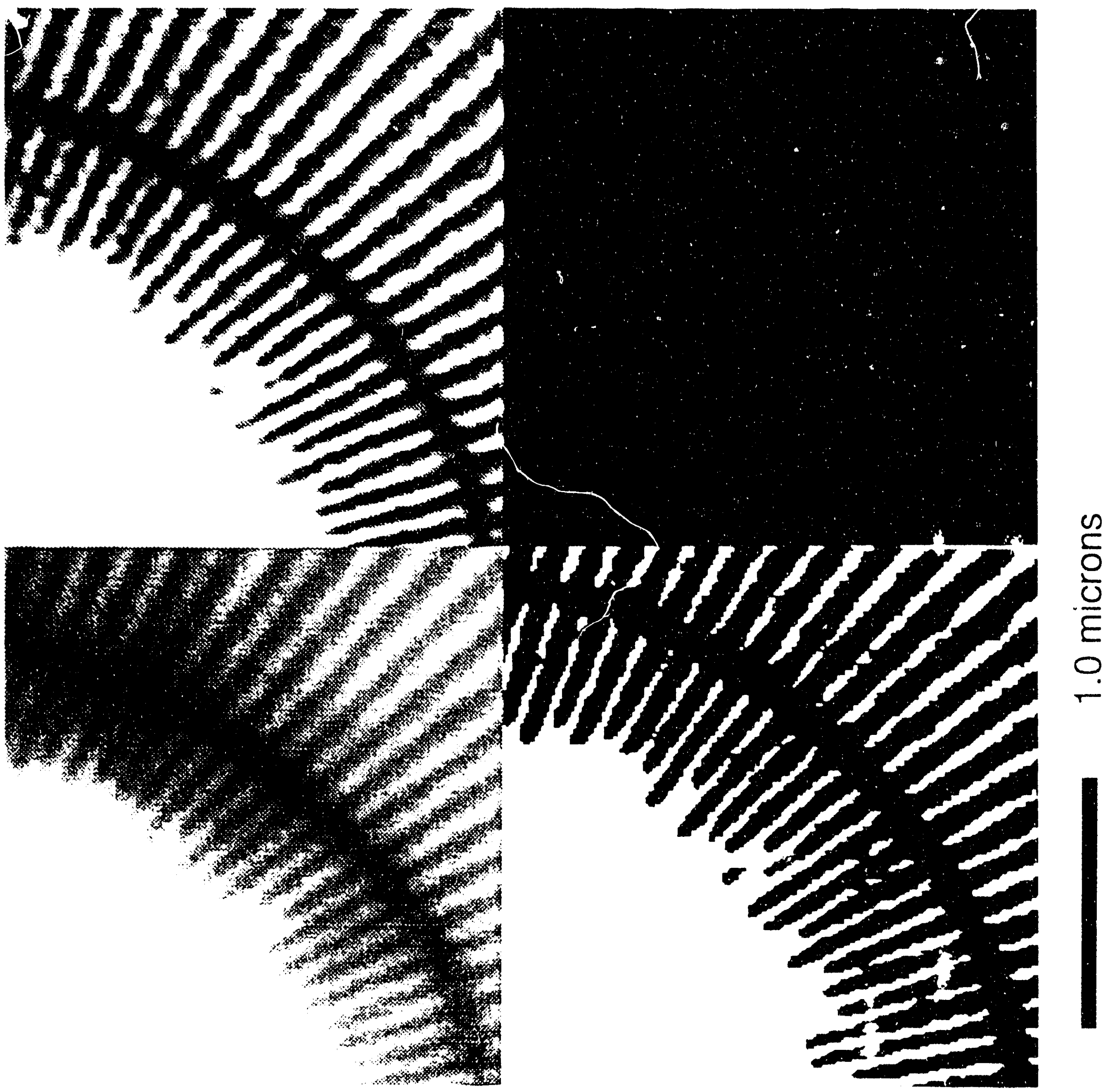

ALS U3.9 undulator
NSLS X-1 undulator
APS undulator A
NSLS X-ray bend
Coherent flux (ph/sec/0.1% BW)
Wavelength (nm)
10^14
10^12
10^10
10^8
10^6
0.1
1.0
10.0


Zoneplate 100 nm Ni, δ_{rN}=45 nm
Diffraction efficiency
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
Wavelength in nm
1.5
2
2.5
3
3.5
4
4.5
5
O
N
C

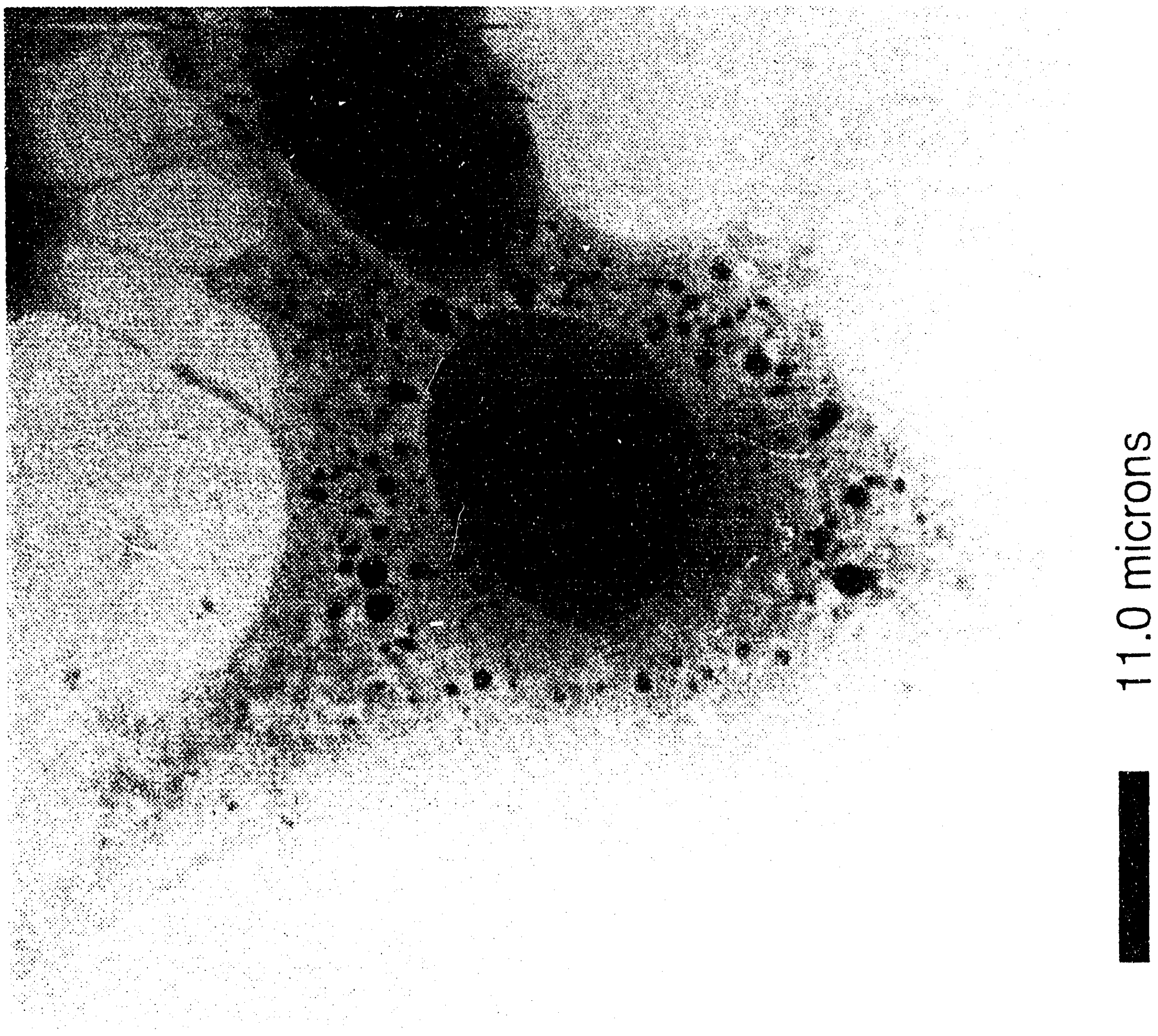


Zone Plate: 100 nm Ni, δrN=45 nm
Modulation transfer function
Spatial frequency f in μm⁻¹
Theory:
Vert.
Horiz.
Data:
Vert.
Horiz.
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0
5
10
15
20
25

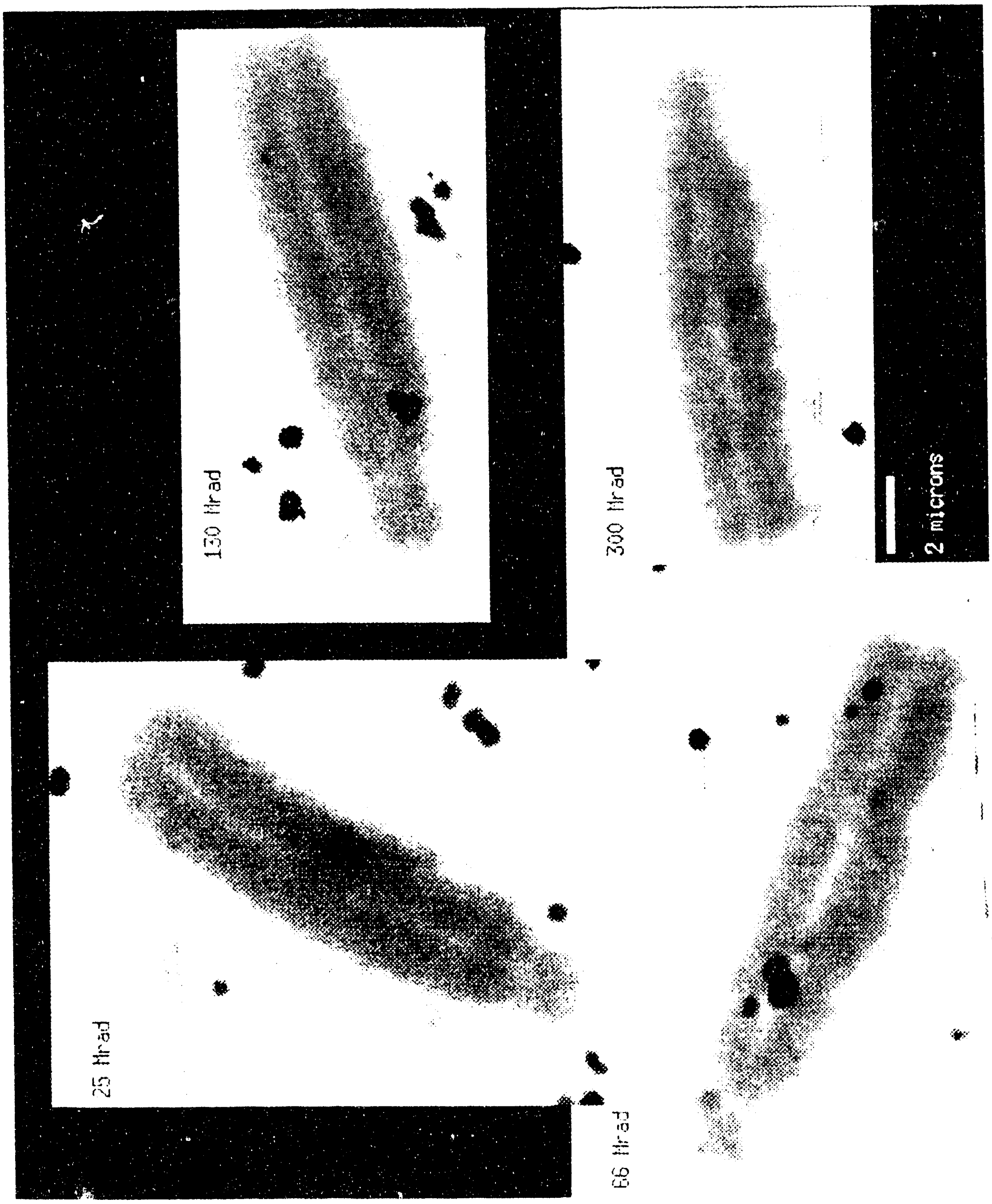

5.0 microns
cj128st3.ps

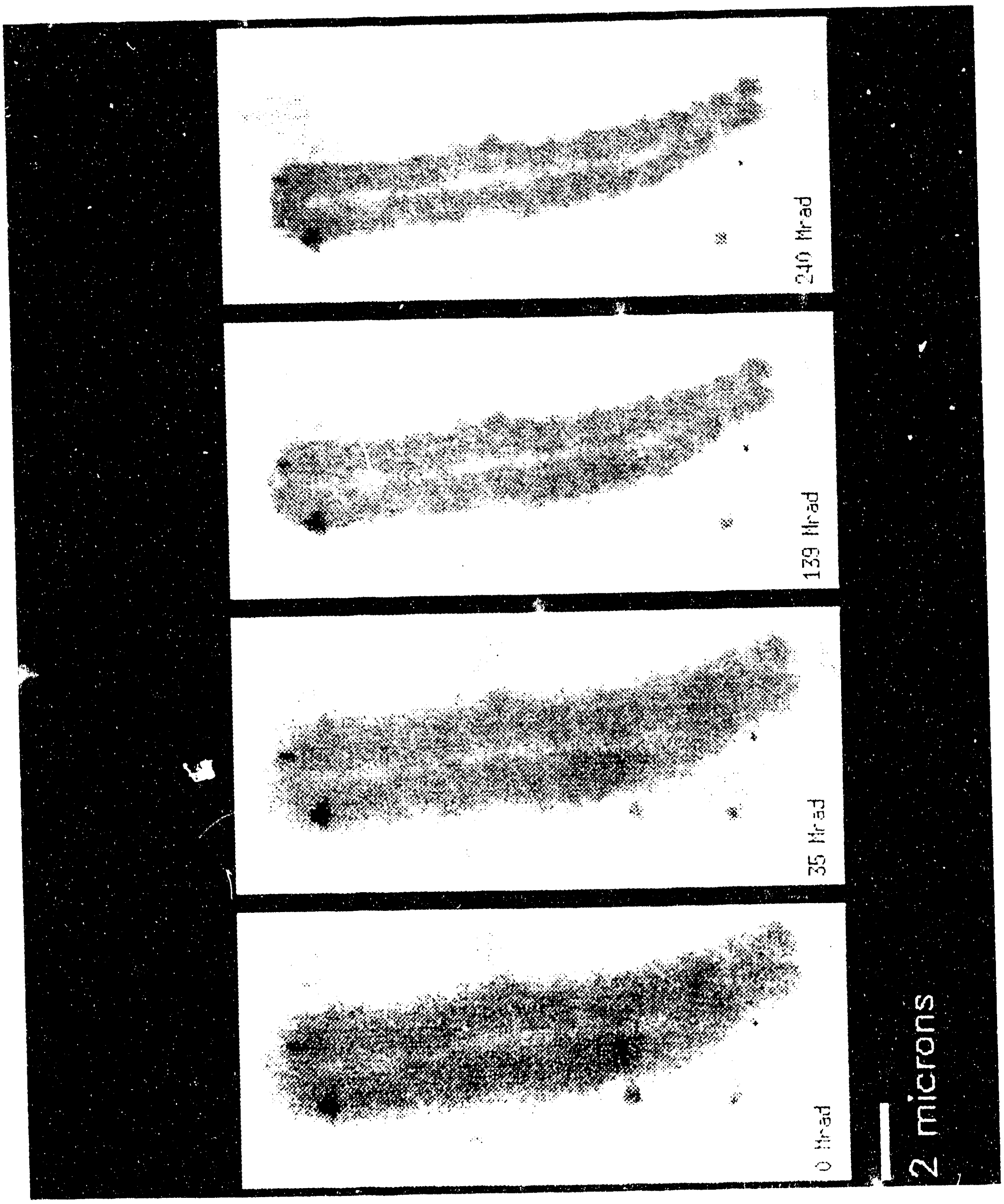


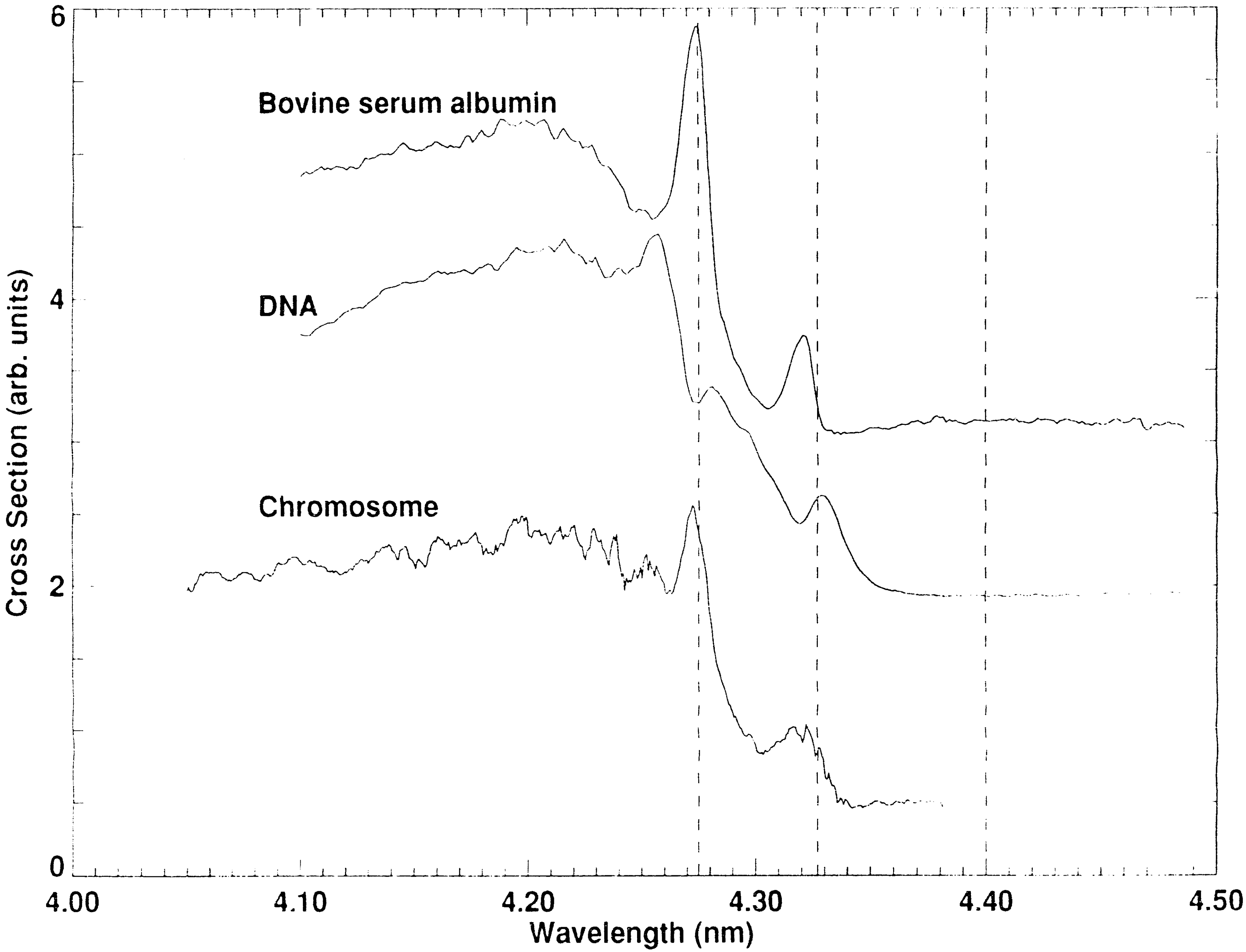
Au test obj. (STEM/STXM/Deconv.)



JU56 (wallabee) cell line


25 Mrad
66 Mrad
130 Mrad
300 Mrad
2 microns

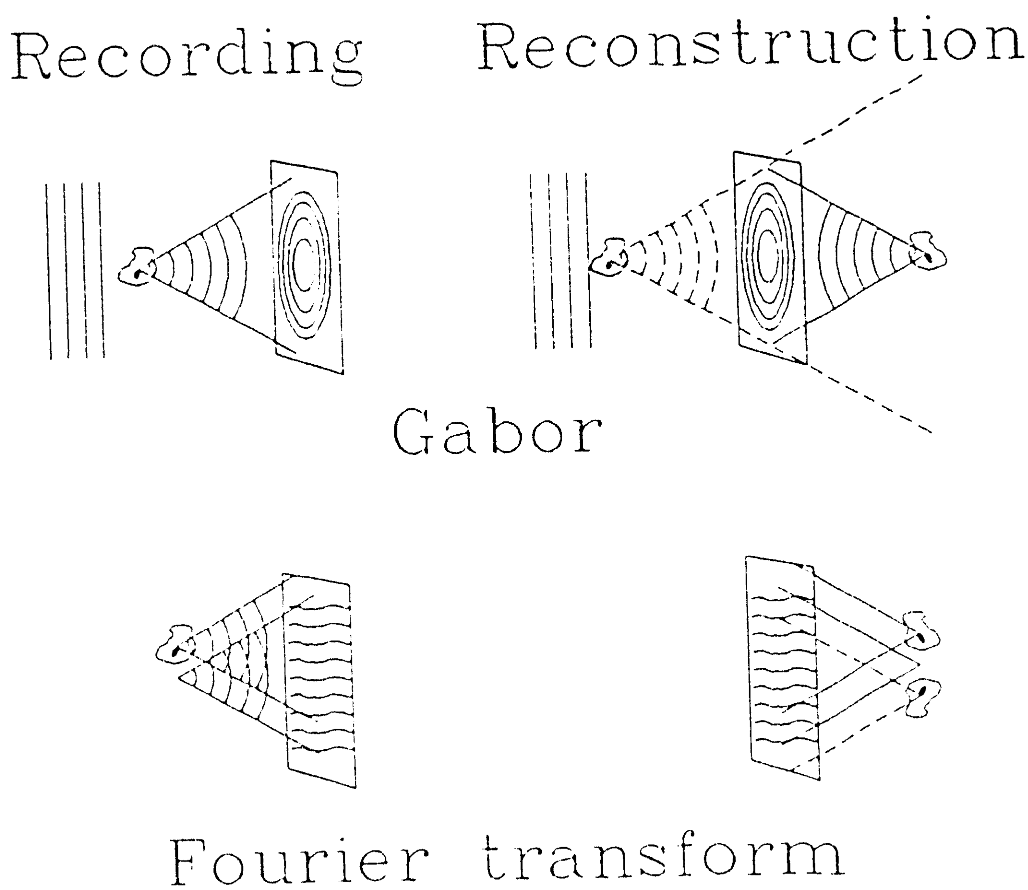

0 Mrad
35 Mrad
139 Mrad
240 Mrad
2 microns

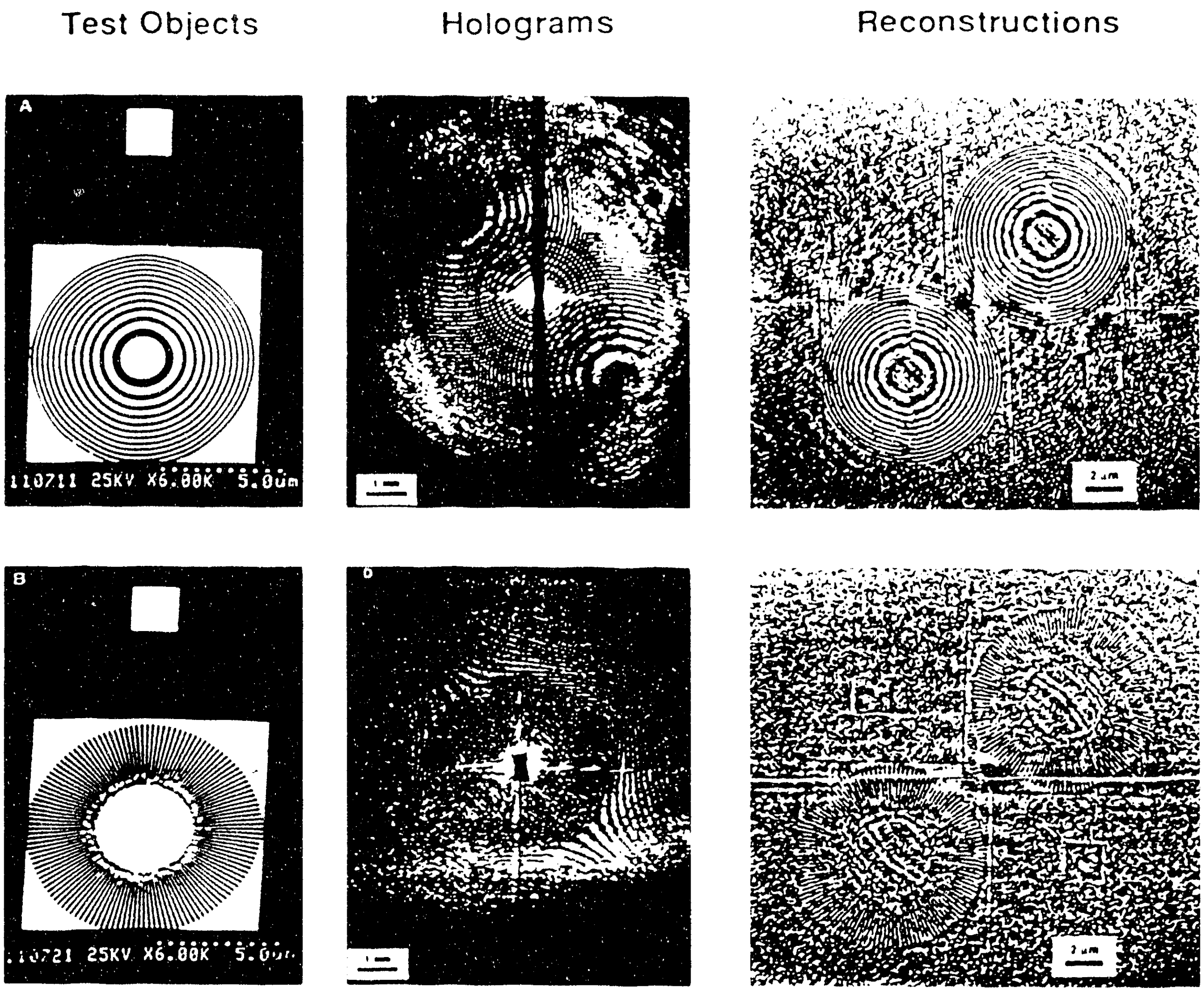


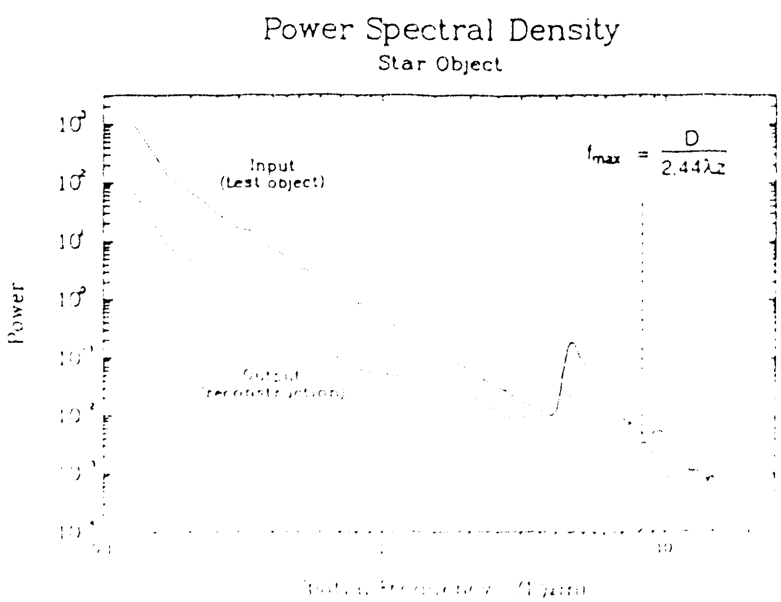
Bovine serum albumin
DNA
Chromosome
Cross Section (arb. units)
Wavelength (nm)
0
2
4
6
4.00
4.10
4.20
4.30
4.40
4.50

Holography: microscopy by wavefront reconstruction

- Interfere the wave scattered from an object with a reference wavefront.
- Illumination of the processed hologram by the reference wavefront recreates the object wavefield.
- Two geometries are well-matched to the current status of x-ray sources, optics, and detectors: Gabor and Fourier transform.




Test Objects
Holograms
Reconstructions
A
110711 25KV X6.00K 5.0um
B
2 um


Power Spectral Density
Star Object
Input
(test object)
Output
(reconstruction)
$f_{max} = \frac{D}{2.44\lambda z}$
Power

Hologram readout: from TEM to SFM

Transmission electron microscope:

- measures thickness variations of photoresist, derivative of fringe profile (metal shadowing)
- destructive to resist
- spiral distortions on TEM limit effective hologram numerical aperture (thus image resolution)
- metal grain, multiple scattering, mass loss limits resolution to ~ 10 nm
- requires resists on thin windows (durability)
- multiple steps to digitized hologram (metal shadowing, TEM photographs, scanning microdensitometer **OR** contact print & PC-based page scanner)

Scanning force microscope (van der Waals force rather than quantum mechanical tunnelling):

- measures surface profile of photoresist
- nondestructive (mostly)
- potential for atomic resolution
- field distortion can be made negligible
- direct digital readout

AFM readout: David Abraham
IBM T.J. Watson Research Center

← 5 μm →

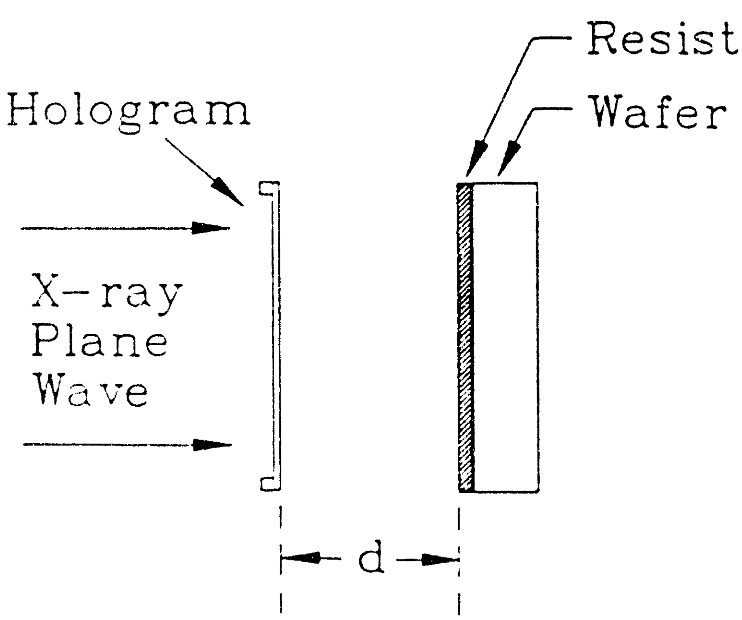
$(5\ \mu m)^2$ 512^2 pixels

293 Å pixels

Computer generated holograms for projection x-ray lithography

- Holographic optical elements serve as single element aberration-corrected optics
- Fabrication requirements: equal resolution and registration as is required for proximity x-ray lithography
- The mask–wafer gap can be 50–1000 μm
- Recording geometry and illumination requirements appear to be compatible with existing x-ray steppers at synchrotron light sources.
- High depth-of-field: $4\delta_t^2/\lambda \approx 10\ \mu$m
- Especially high degree of immunity to image corruption caused by moderate non-localization of information

But twin image?

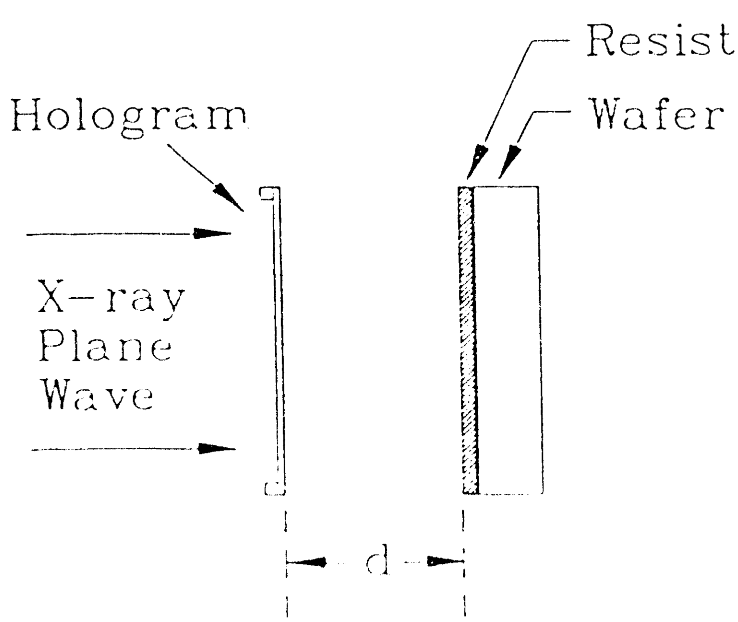


Technique for printing a noise-free image

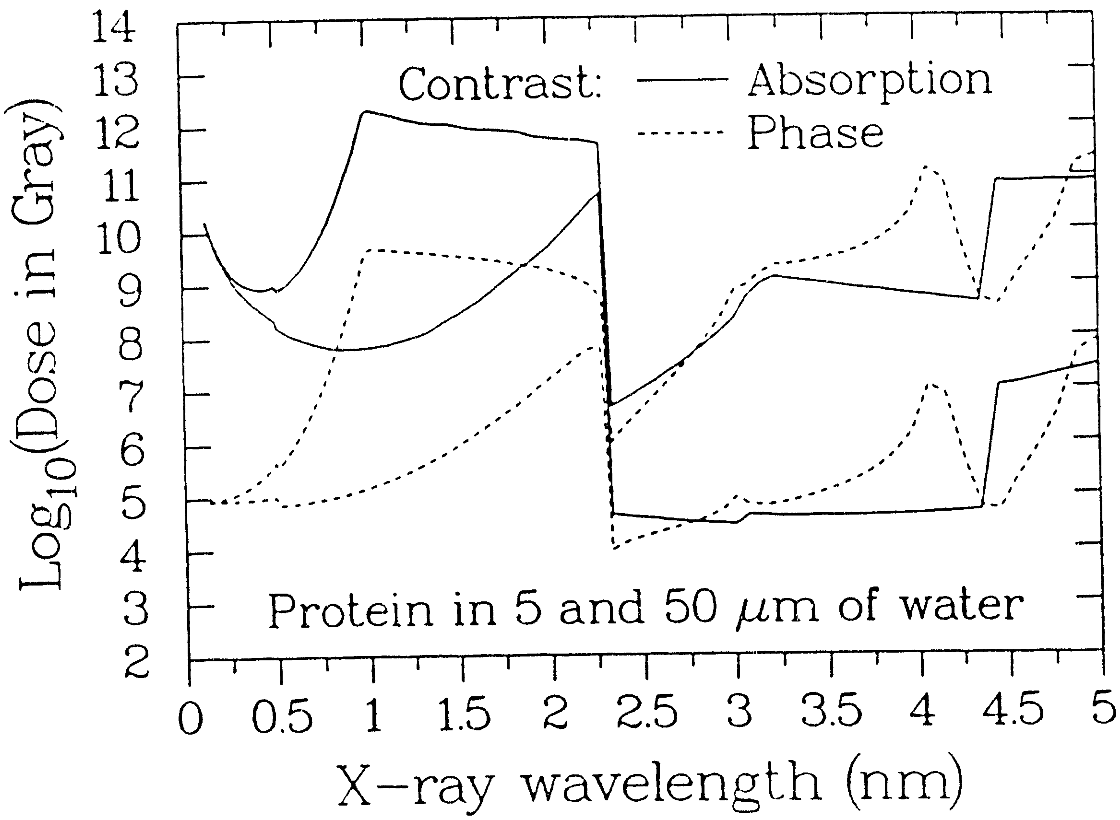
Use x-ray refractive index $n_r = 1 - \delta - i\beta$ and $\psi = \exp(-ikn_r t)$ for a material thickness t (get δ, β from Henke).

1. Backpropagate the desired wavefield from the wafer to the hologram.
2. At the hologram, pick t at each pixel to match the phase exactly and the amplitude approximately (ANOMALOUS DISPERSION!!!!)
3. Forward propagate the wavefield back to the wafer. Re-impose the desired intensity levels but leave the phase untouched.
4. Repeat steps 1–3 til convergence

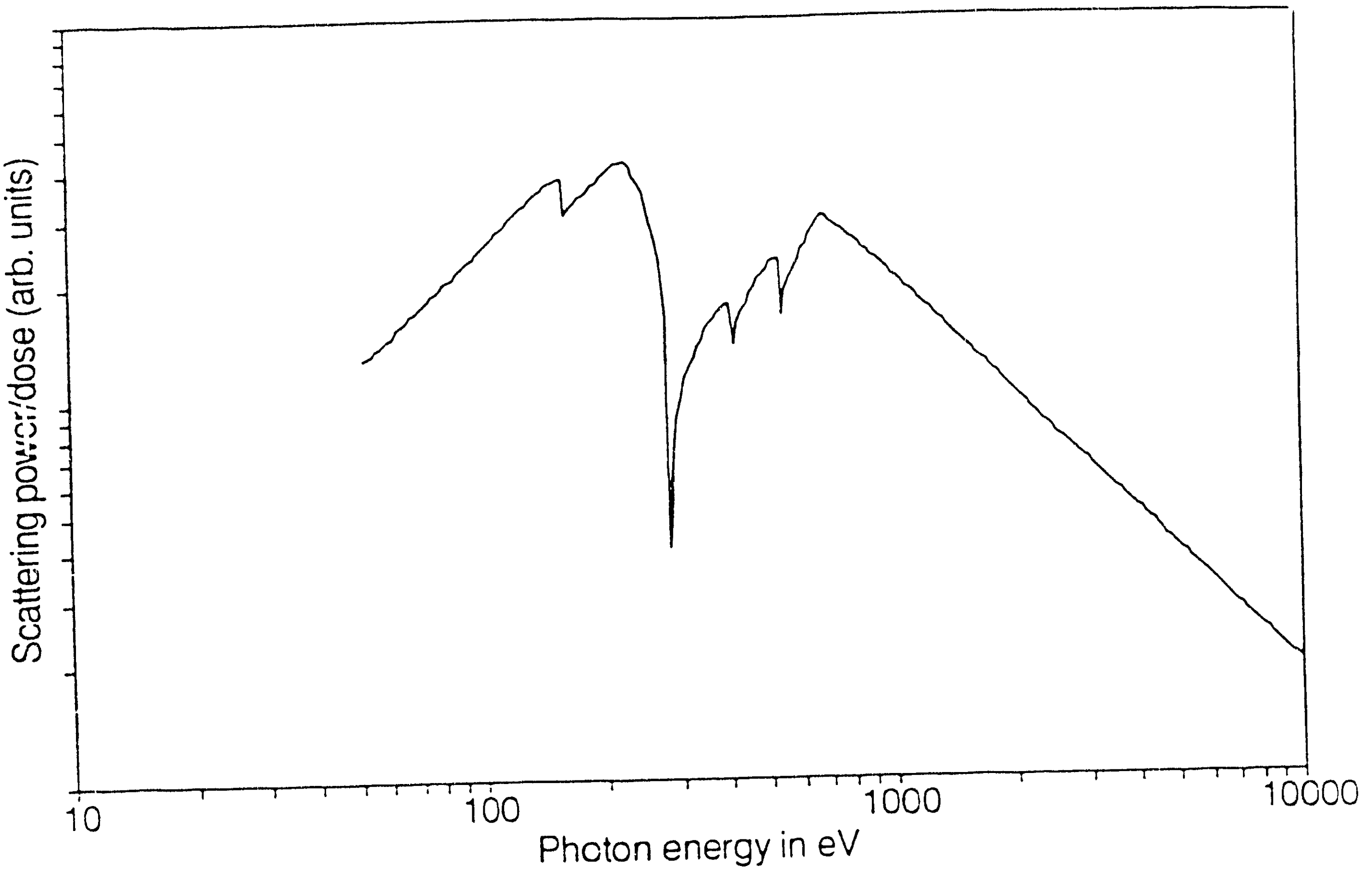
The key is that we have a free parameter on each side of the problem (the optical phase at the wafer, and the material thickness at the hologram). See results of simulations.



Calculated dose



Scattering/dose for <= 1 micron protein



$$\frac{\text{scattering}}{\text{dose}} \sim \frac{(f_1^2+f_2^2)\cdot(\delta_t^2\,\mu_e^{-1})^2}{(\delta_t^2\,\mu_e^{-1})}$$

$$\sim (f_1^2+f_2^2)\,\delta_t^2\,\lambda f_2$$

Making zone plates harder

Fresnel zone plate zones should either be

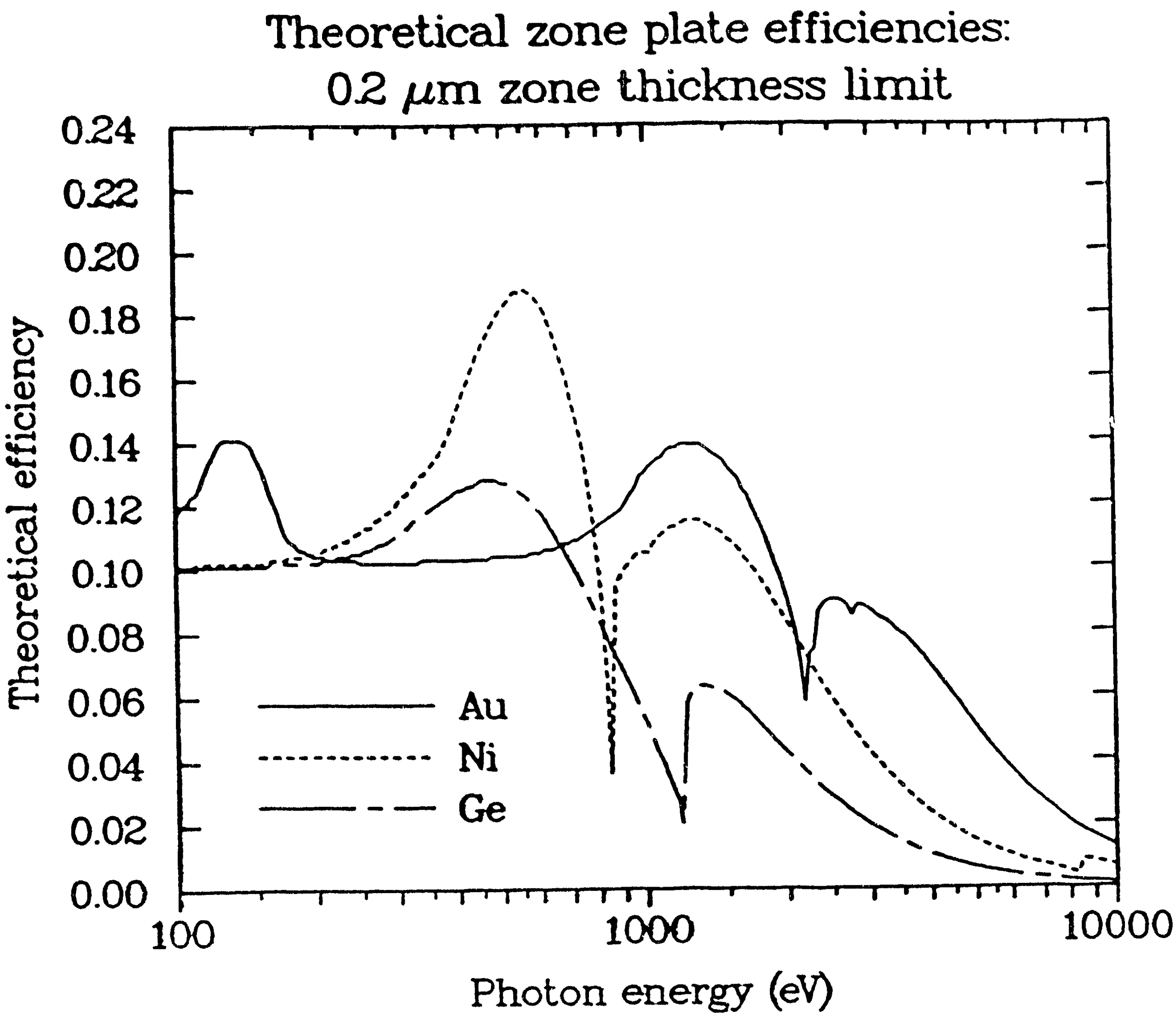
- Opaque
- Phase shifting (π)

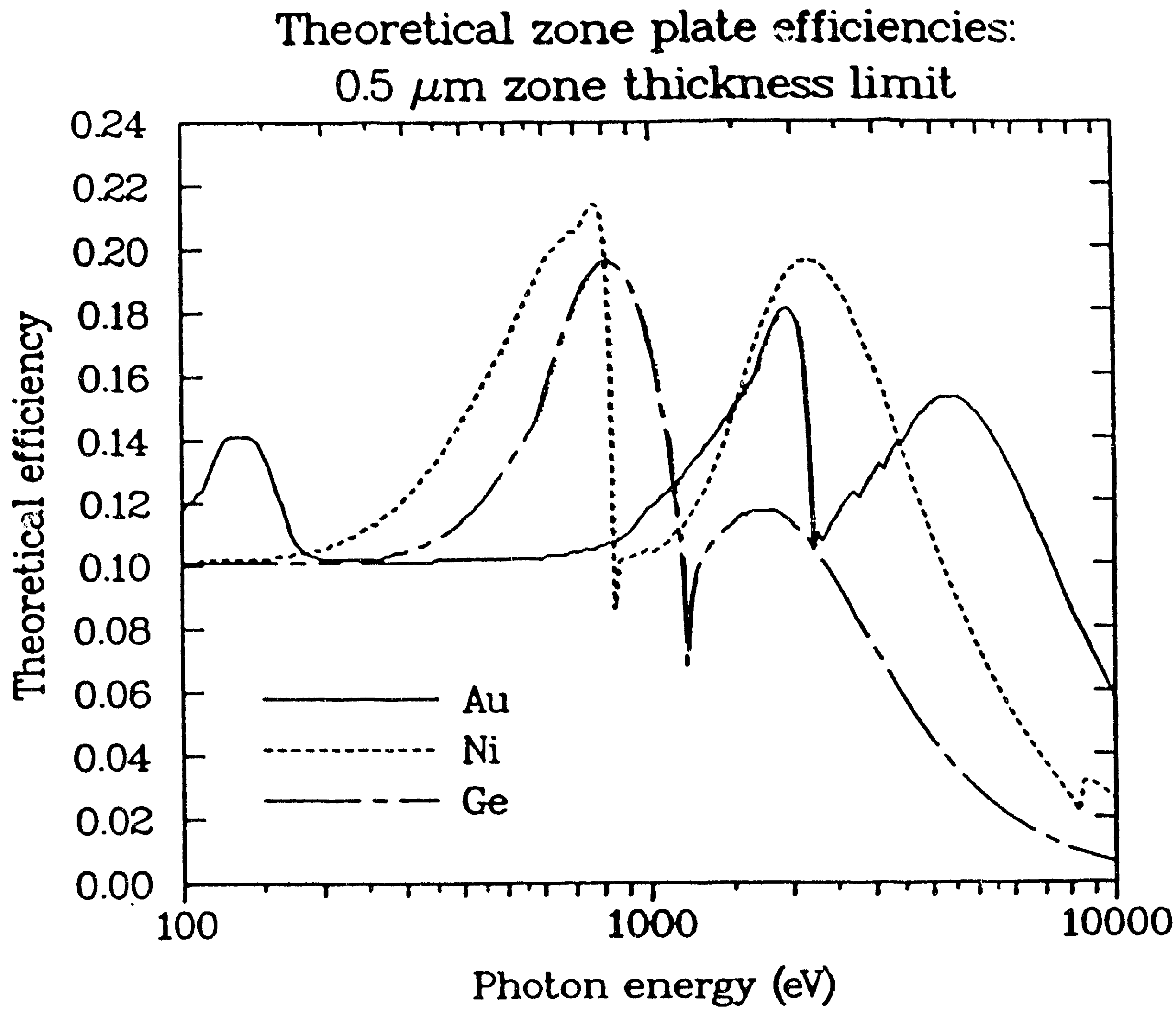
Zone plate efficiency ϵ

$$\epsilon \simeq \frac{1}{\pi^2}[1 + \exp(-\frac{4\pi}{\lambda}\beta t) - 2\exp(-\frac{4\pi}{\lambda}\beta t)\cos(\frac{4\pi}{\lambda}\delta t)]$$

Making e.g., 0.05 μm wide, 0.5 μm high zones is difficult.

- E-beam lithography in resist
- Sputter & slice


Theoretical zone plate efficiencies:
0.2 μm zone thickness limit
Theoretical efficiency
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
Au
Ni
Ge
100
1000
10000
Photon energy (eV)



Theoretical zone plate efficiencies:
0.5 μm zone thickness limit
Theoretical efficiency
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
Au
Ni
Ge
100
1000
10000
Photon energy (eV)

HIGH-RESOLUTION SCATTERING WITH COHERENT X-RAYS AND X-RAY INTENSITY FLUCTUATION SPECTROSCOPY

Brian Stephenson
IBM Research Division
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The use of coherent incident radiation in a scattering measurement provides a wealth of information about the disorder present in the sample which cannot be obtained using incoherent radiation. In general, the scattering of a coherent incident beam produces a "speckle" pattern whenever the sample contains randomly distributed regions which scatter differently. If the arrangement of the regions evolves with time, the speckle pattern will also change. Observation of the intensity fluctuations at a single point in the speckle pattern, a technique known as intensity fluctuation spectroscopy, has been widely used with visible light to study processes such as critical fluctuations near phase transitions in fluids and the diffusion of particles in liquids. Using visible light, it is not possible to study length scales less than about 200nm, or opaque materials. However, by using coherent x-rays, the dynamics of processes involving atomic length scales can be observed in a wide range of materials. In this talk I will report on progress in the development of x-ray intensity fluctuation spectroscopy (XIFS). In our initial work,[1] we produced a coherent x-ray beam of 0.15nm wavelength by using a pinhole a few microns in diameter and a high-brilliance synchrotron source. We used this beam to observe an x-ray speckle pattern in the diffraction from anti-phase domains in a single crystal of Cu_3Au. In a subsequent experiment using the APS/CHESS x-ray undulator, we have carried out an XIFS study of the kinetics of ordering in Cu_3Au.[2] Finally, I will discuss the prospects for using XIFS at APS to study the dynamics of disorder having correlation lengths in the 1 to 100nm range, such as diffusion in amorphous systems.

[1] "The Observation of Speckle by Diffraction with Coherent X-rays," M. Sutton, S.G.J. Mochrie, T. Greytak, S.E. Nagler, L.E. Berman, G. Held, and G.B. Stephenson, *Nature* **352**, 608 (1991).
[2] Collaborators: E. Dufresne, M. Sutton, *McGill Univ.*; R. Headrick, *CHESS*; G. Held, *IBM*; S. Mochrie, *MIT*; B. Rodricks, *APS*; C. Thompson, *Polytechnic Univ.*.

High-Resolution Scattering with Coherent X-rays and X-ray Intensity Fluctuation Spectroscopy

New Frontiers at the APS

Brian Stephenson
IBM Research

Collaborators:

Eric Dufresne, Ken Elder, Mark Sutton, *McGill Univ.*

Tom Greytak, Simon Mochrie, *MIT*

Glenn Held, *IBM*

Steve Nagler, *Univ. of Florida*

Carol Thompson, *Polytechnic Univ.*

Lonny Berman, *National Synchrotron Light Source*

Randy Headrick, *Cornell High Energy Synchrotron Source*

Brian Rodricks, *Advanced Photon Source*

OUTLINE

- Scattering with coherent light
  - > *Resolution and Coherence*
  - > *Speckle from Disordered Systems*
  - > *Intensity Fluctuation Spectroscopy*
  - > *Opportunities with x-rays: atomic-scale dynamics and structure*

- Producing a coherent x-ray beam
  - > *Source brilliance*

- Measurement of speckle from anti-phase domains in Cu_3Au
  (*Nature* **352**, 608 (1991))

- Prospects for Intensity Fluctuation Spectroscopy at APS

Resolution and Coherence

Scattering with a coherent beam ⇒

Coherence length as large as sample size

$$d_{coh} \geq L$$

Equivalent to:

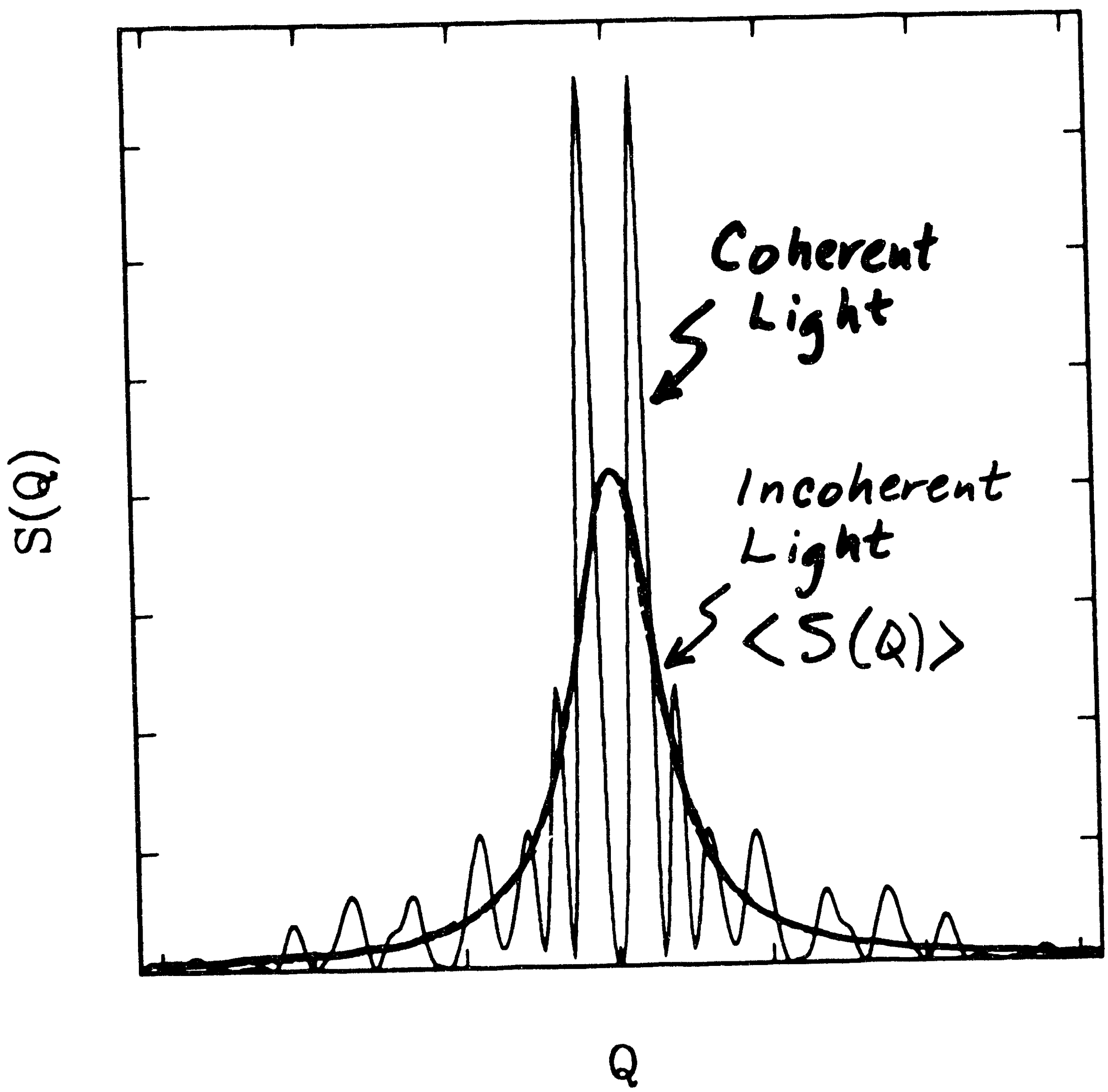
Wavenumber uncertainty small enough to resolve correlations as large as L

$$\Delta q \leq \frac{2\pi}{L}$$

or, high angular resolution

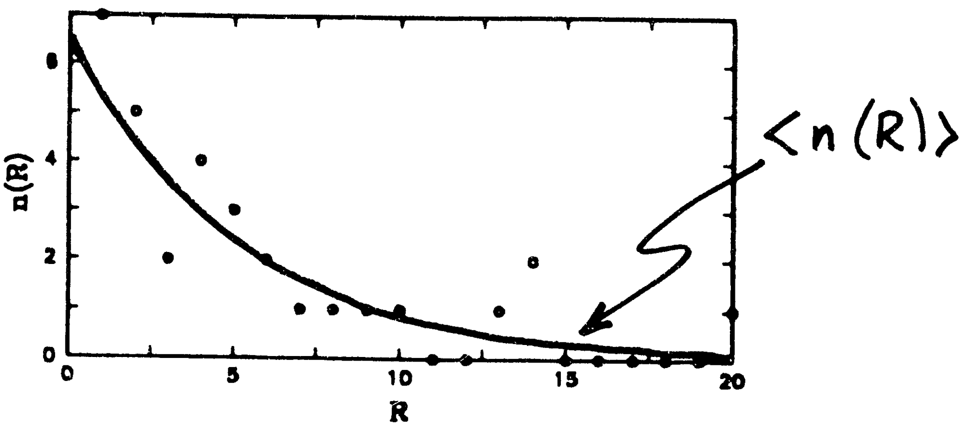
$$\Delta \theta \leq \sim \frac{\lambda}{2L}$$

Scattering from a Disordered System

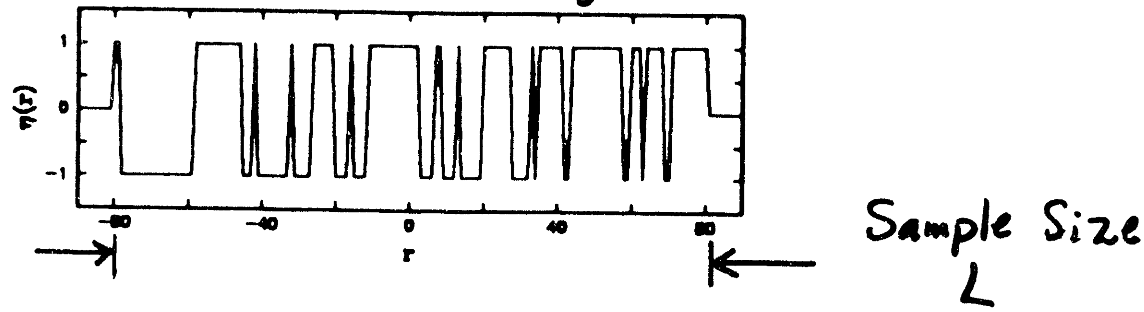


- Speckle pattern depends on exact arrangement of domains, not just domain size distribution
- If incident light is not coherent, resolution is insufficient to observe speckle pattern

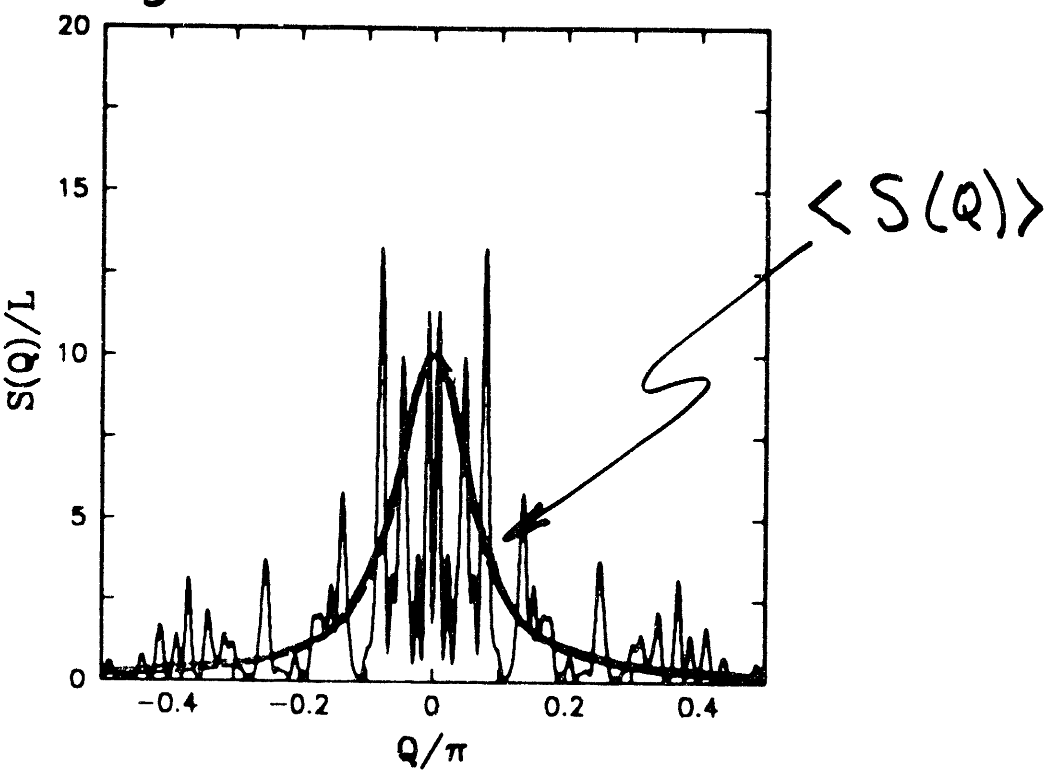
Domain Size Distribution:



An Actual Domain Arrangement:



Scattering Pattern from Domains:



Intensity Fluctuation Spectroscopy

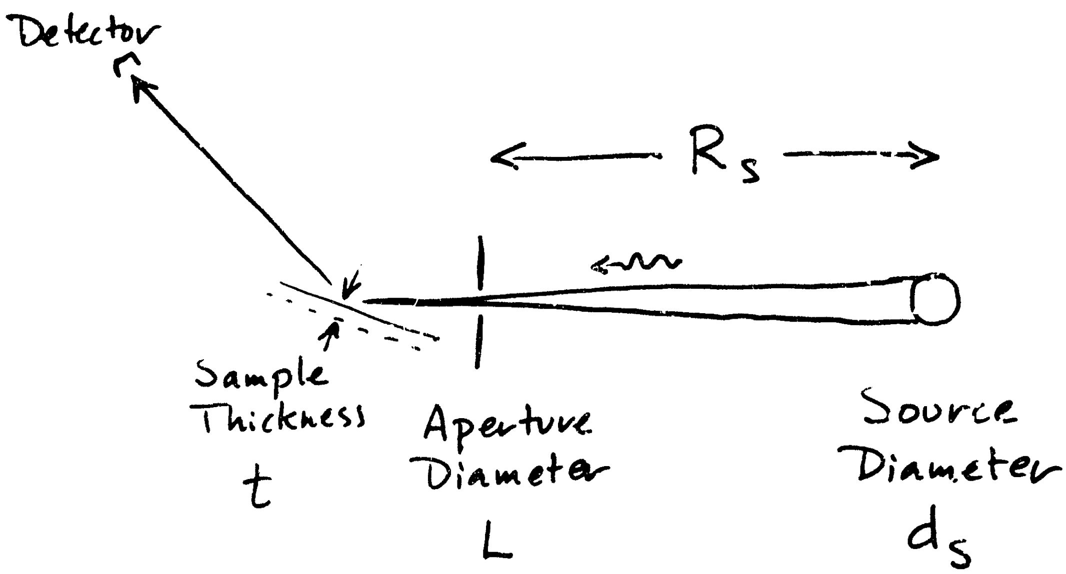
- Well-developed technique using visible light (lasers)
- Used to study dynamics of processes such as
  - density fluctuations near critical points
  - diffusion of particles in fluids

- Visible light cannot be used for $Q > \dfrac{4\pi}{(\lambda = 4000\mathring{A})}$
- Use of x-rays ($\lambda = 1\mathring{A}$) would allow study of dynamics of atomic-scale fluctuations:
  - order in alloys, liquid crystals, etc.
  - charge density waves
  - quasicrystals
  - diffusion of defects

- Such dynamics can not be studied by conventional time-resolved scattering with incoherent x-rays, which is sensitive only to the ensemble average

Use of Incoherent X-ray Source:

Resolution / Coherence Requirements for Incident Beam



$$L \leq d_{coh} \equiv \frac{\lambda}{2} \frac{R_s}{d_s}$$

$$2t\sin\theta \leq \ell_{coh} \equiv \frac{\lambda}{2} \frac{\lambda}{\Delta\lambda}$$

Coherent Light from an Incoherent Source

Longitudinal coherence length:

$$\ell_{coh} = \frac{\lambda}{2}\,\frac{\lambda}{\Delta\lambda} \qquad 0.6\ \mu m\ \text{typ.}$$

Transverse coherence length:

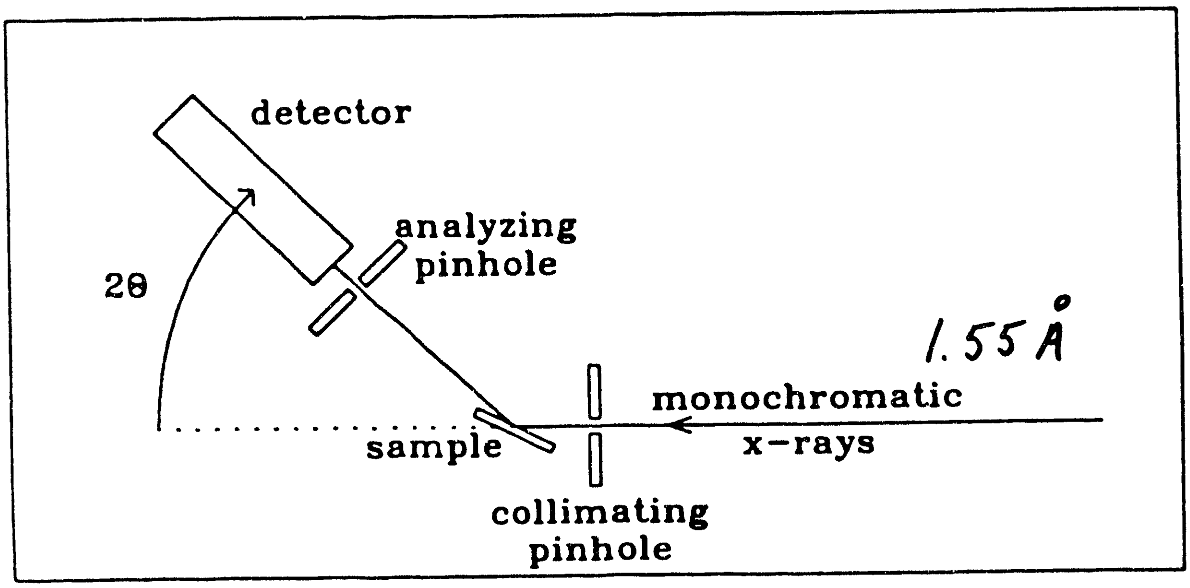
$$d_{coh} = \frac{\lambda}{2}\,\frac{R_{source}}{d_{source}} \qquad 10\ \mu m\ \text{typ.}$$

Transversely coherent flux:

$$F_{coh} = \left(\frac{\lambda}{2}\right)^2 \times \textit{Brilliance}$$

1.24 Å X-ray Source:	NSLS Wiggler	CHESS Undulator	APS Undulator
Brilliance (ph/s/mm2 /mrad2/$10^{-4}\Delta\lambda/\lambda$)	3×10^{14}	3×10^{15}	1.5×10^{17}
F_{coh} (ph/s/$10^{-4}\Delta\lambda/\lambda$)	1.2×10^{6}	1.2×10^{7}	6×10^{8}

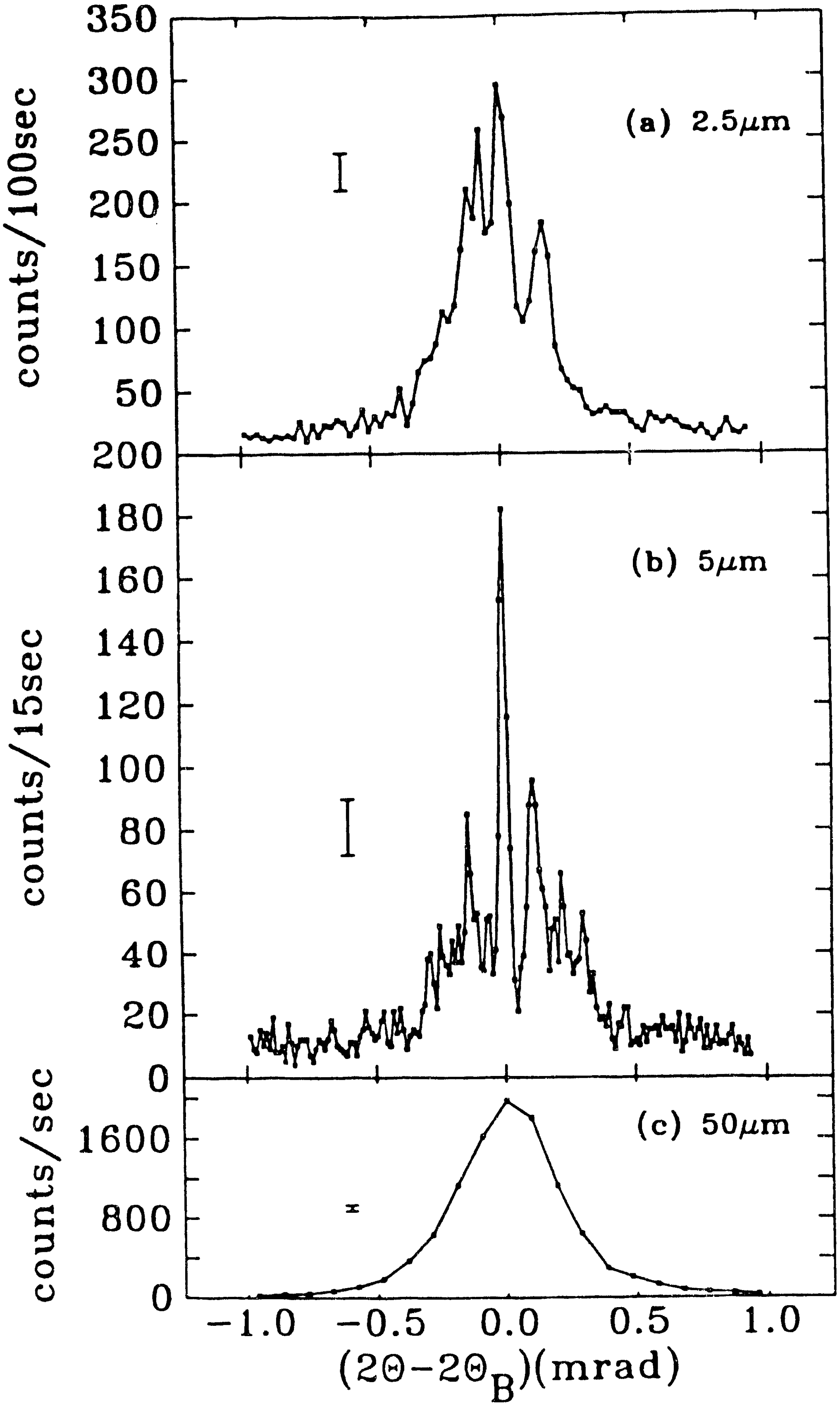
Scattering Geometry using micron-sized pinholes



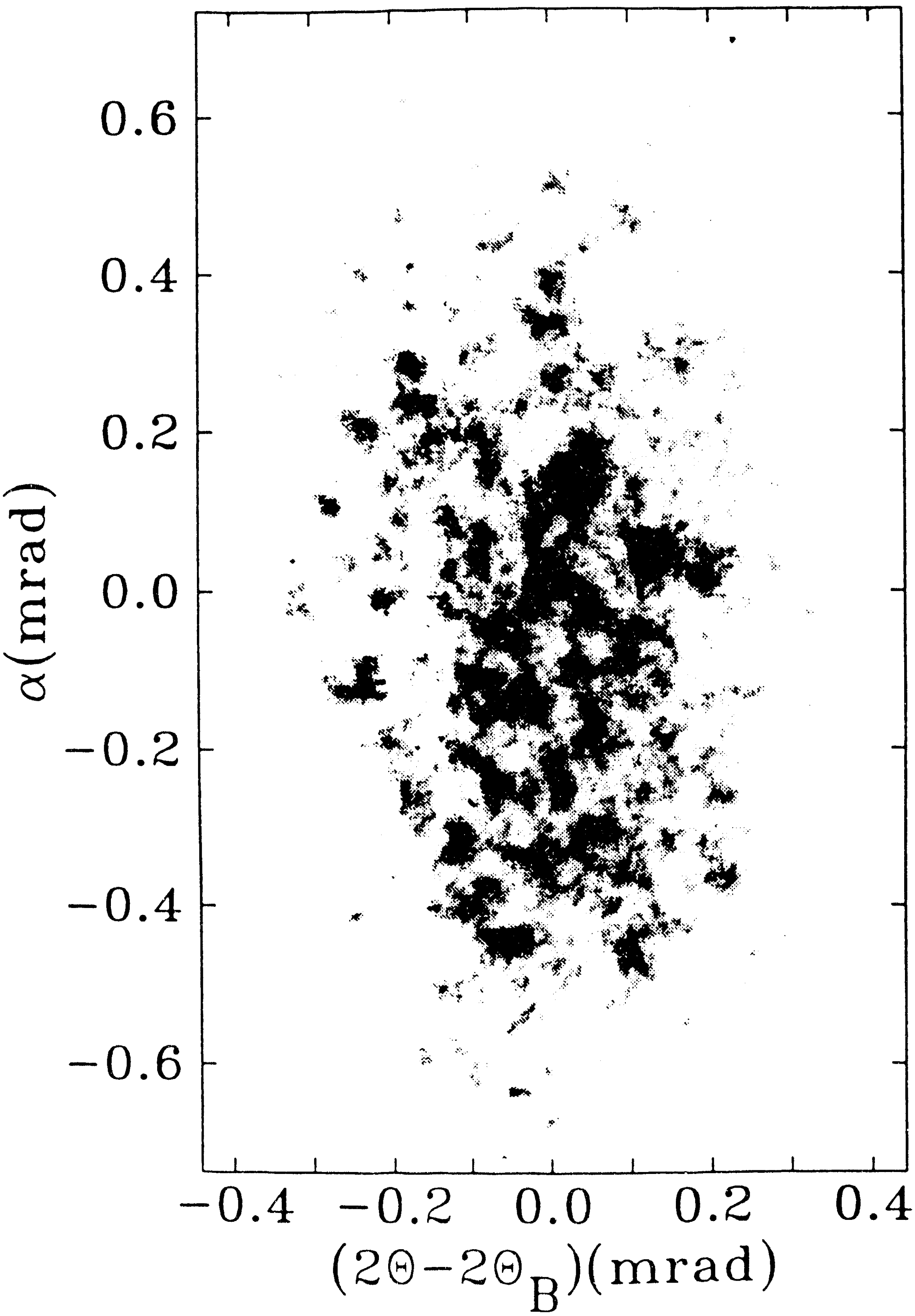
Analyser resolution:

each "speckle" subtends $\Delta(2\theta) \doteq \frac{\lambda/2}{L}$

For $L = 5\,\mu m$, $\Delta(2\theta) = 15\,\mu rad$



350
300
250
200
150
100
50
counts/100sec
(a) 2.5μm
200
180
160
140
120
100
80
60
40
20
0
counts/15sec
(b) 5μm
1600
800
0
counts/sec
(c) 50μm
−1.0
−0.5
0.0
0.5
1.0
(2Θ−2Θ_B)(mrad)


0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
α(mrad)
−0.4
−0.2
0.0
0.2
0.4
(2Θ−2Θ_B)(mrad)

Science with X-ray IFS at APS

Correlation Lengths ξ 10 - 1000 Å

Sample (Beam) Sizes L 0.1 - 10 μm

⇒ Dynamics of SRD in Alloys,
Diffusion in Amorphous Systems,
Dynamics of Displacive Transitions,
Liquid Crystals, Quasicrystals, Surfaces

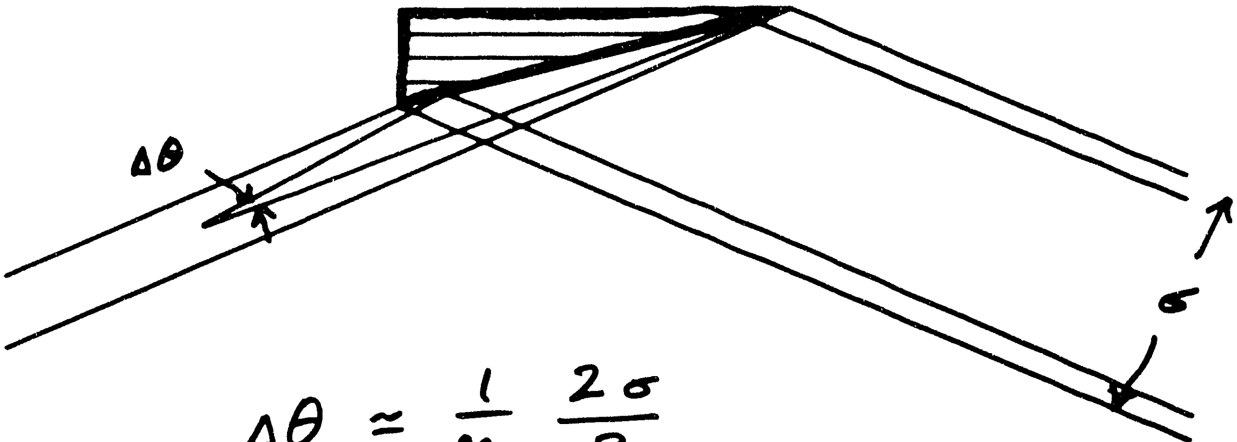
Typical Signal Levels:

	ξ (Å)	L (μm)	Signal (cps)
Single Crystals	1000	10	10^3
(e.g. SRD in	100	1	10^2
order-disorder)	10	0.1	10
Amorphous Material	10	0.1	1

Need Optics to Tailor Coherence Volume

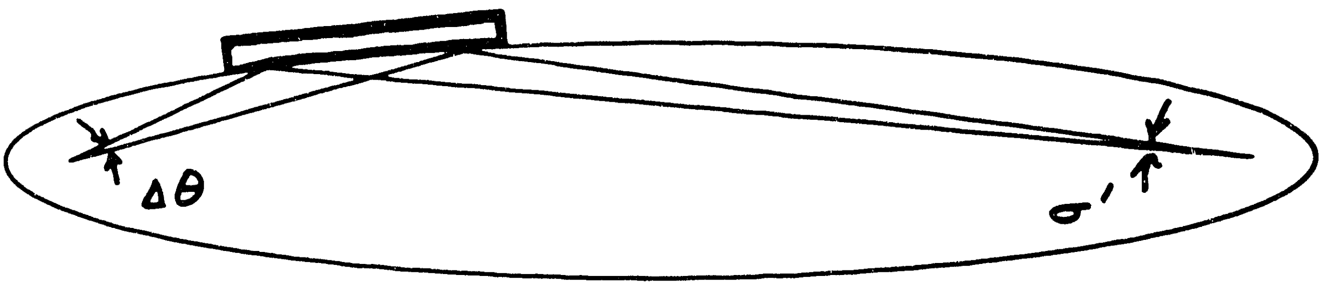
Divergence ↔ Spot Size

Asymmetric Crystal



$$\Delta\theta \simeq \frac{1}{M}\,\frac{2\sigma}{R}$$

Focussing Optic (Mirror / Zone Plate)



$$\Delta\theta \simeq \frac{1}{M}\,2\sigma'$$

Need Optics to Tailor Coherence Volume

APS Undulator A

		Vertical	Horizontal	
Source size	2σ	170	600	μm
Divergence	$2\sigma'$	18	48	μrad

d_{coh} ($\lambda = 2Å$)	$\Delta\theta$	DeMagnification Vertical Xtal @ 60m	Vertical Focussing Optic	Horizontal Xtal @ 60m	Horizontal Focussing Optic
μm	μrad				
30	3	<u>1:1</u>	–	–	–
10	10	3:1	(1:2)	<u>1:1</u>	–
1	100	<u>30:1</u>	5:1	<u>10:1</u>	2:1
0.1	1000	(300:1)	<u>50:1</u>	(100:1)	<u>20:1</u>

$\Rightarrow$ Optics in or near hutch

ADVANCED PHOTON SOURCE: TECHNICAL DEVELOPMENTS

Top-up Operation of APS

John N. Galayda

Fifth Users Meeting
October 13-15, 1992

Top-up Operation of APS

Definition of top-up

Immediate advantages

Immediate issues for utilization

- Personnel protection
- Chamber protection
- Beam stability
- Beam utilization

Long - term advantages

Long - term issues for utilization

John N. Galayda

Top - up Operation of APS

Definition of essentials:

Injection with
Insertion devices closed
Shuttters open
Beam stability specifications met
(except during a short time interval dt)

Negotiable parameter:

dT, injector repetition period; 0.5 seconds minimum

If beam lifetime is T, and current is I, then the variation in stored current is

$$dI = I\ (dT/T)$$

Advantages of Top - up Operation
(From presentation by D. Moncton @ 4th Gen workshop)

Experiments continue during injection - shutters open, undulators closed

Achieve "constant current" operation

e.g., I = 100 mA, T = 40 hrs, dT = 1 minute

dI = 0.04 mA

Current is stable to better than 0.1%

Improves stability of storage ring
Improves stability of optics
Maximizes available beam intensity
Eliminates changing S/N ratio
Minimizes nonlinear monitor effects

Personnel Protection

Bremsstrahlung in hutches during injection with shutters up?

MCI 183 mrem for total loss of 300 mA in an ID chamber (H. J. Moe, APS-LS-141, revised)

Analyze credible trajectories of stored beam, incoming beam during injection process

Investigation of safety of following operation rules:

Shutters closed during fill from zero current with high charging rate

Inhibit injection if stored beam is lost, shutters up

Inhibit injection if incoming beam charge is too large

Issues still under study

General radiation environment- increased simply because average current = maximum current- Same dose per amp-hour of beam

Chamber Protection

@ APS, mis-steered beam must be aborted in 1 millisecond, top-up or not

Extra effort to prevent disruption of feedback orbit control by injection process

Vertical beam blowup for a short time after injection would be invisible to a typical RF beam position monitor - damping Time 9 msec

ESRF to add beam size measurement to the chamber protection logic

APS to enlarge ID radiation exit port aperture-EDM channel in beam pipe

Beam Stability

Synchrotron, betatron feedbacks should be OK

Orbit control feedbacks - care must be taken to insure loop stability

Efforts will be made to minimize disturbance of stored beam, to reduce potential of problems from items above; eg,

Try to limit mismatch of injection bumps to no more than 0.17 mm increase in beam size;

Beam will damp to within 5% of nominal size in about 22 milliseconds

Beam Utilization

Data inhibit signal supplied to beamlines

Realtime monitoring of beam current, profile

Experiment compatibility with frequent changes in current

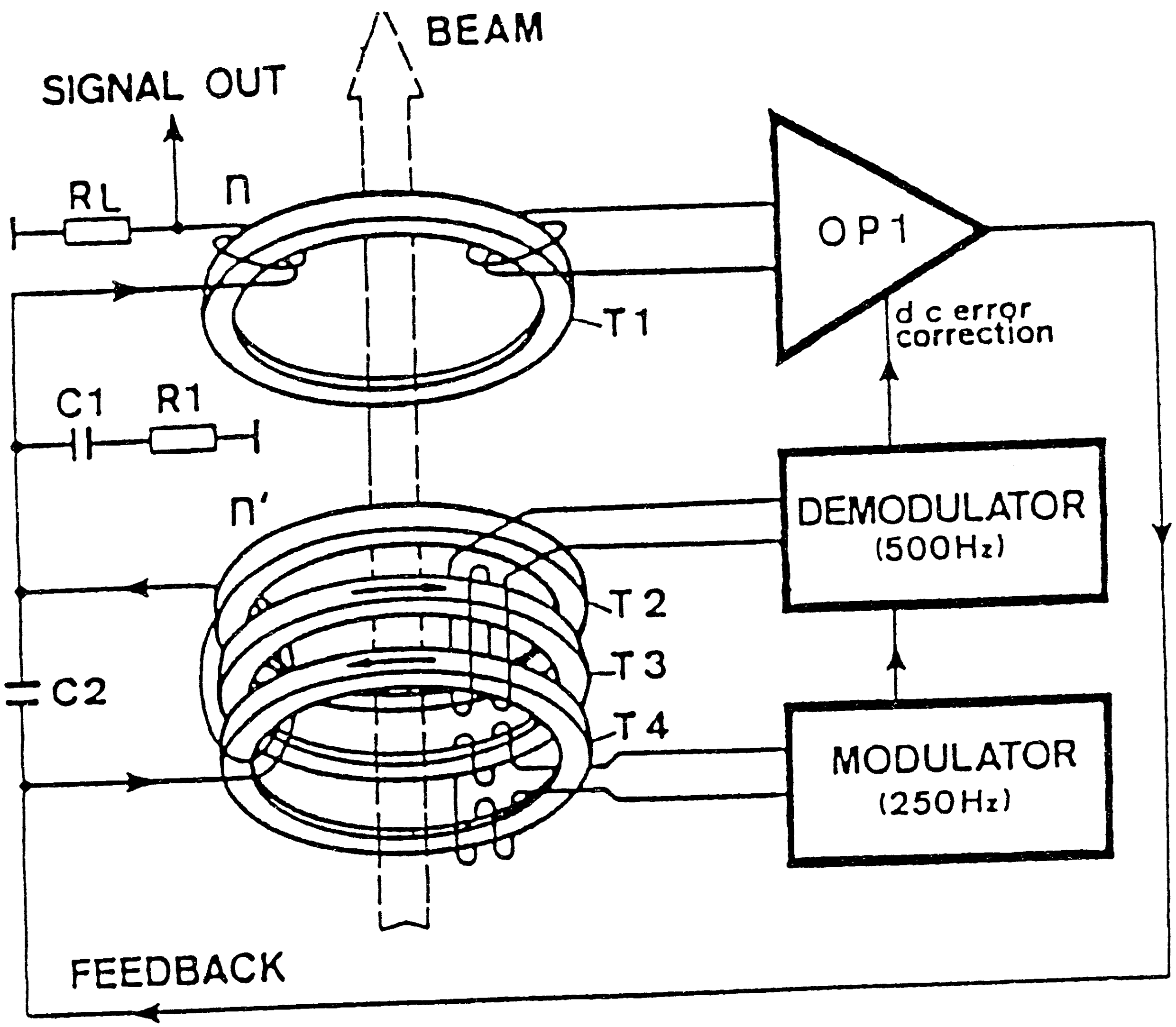
Can one trust an Io monitor and a beamsize monitor at the endstation, compatible with experiments?

Charged-particle diagnostic techniques:

Beam current to better than 0.1% of full scale

Beam profile to better than 25 microns, non-intercepting, visible light

Scanning aperture or filament: 5 microns or better



Schematic of Parametric Current Transformer

Julien BERGOZ
Crozet, 01170 Gex, France
Tel. (33) 50.41.00.89
Fax (33) 50.41.01.99

Price list

Parametric Current Transformer for use as beam monitor in particle accelerators

2.0 Parametric current transformer simplified version

Available now

single range, full scale:	-250 mA ... 0 ... +250 mA
offset ranges	-500 mA ... 0 -or- 0 ... + 500mA
linearity error	< ± 0.02 % ± zero error
resolution*	< ± 0.020 mA rms
zero drift (1 hour)*	< ± 0.025 mA rms
noise (0 ... 1 kHz)	< ± 0.025 mA rms
modulator ripple (f≈7 kHz)	< ± 3 mA rms
long term dc zero drift	< ± 0.1 mA/month
fequency range	dc .... 20 kHz
output signal	- 10V ... 0 ... +10V
output slew rate	0.1 V / µs max.
built-in calibration source	- 250 mA and +250 mA
absolute accuracy	> ± 0.25 %
built-in self-test function	
*(integration window 1s)	

Sensor dimensions: o.d.	260 mm max.
i.d.	170 mm min. — 6.7" ID
h	80 mm max.
Power requirements:	+ 15 ± 5% Vdc, 100 mA
	- 15 ± 5% Vdc, 100 mA
Regulation:	> ± 0.1 %
Calibration/Offset control:	unipolar switch, user-supplied

Includes:

- one torroid sensor with two 3-meter cables leading to the electronics front-end box
- one front-end electronics box. Dimensions are 185x130x70mm
- one open-ended 3-meter cable leading to the user-supplied power supply, calibration/offset control and monitoring device.

Rings designed to optimize other performance parameters at the expense of lifetime:

B-factories at PEP, CESR

e.g. top-up for 4 seconds every 5 minutes

Synchrotron radiation rings

Louis Emery, 1991 Particle Accelerator Conference pg 1633

E = 4 GeV, emittance 0.025 nanometers, T<5 hours

Beam Utilization

It is easy to design an experiment that depends implicitly on slow, smooth variation of beam current

Countermeasures

- Do complete parameter scans between injection pulses
- Accurate realtime normalization to flux into the beamline
- Full interception of the beam striking sample is highly desirable: practical only for harder X-rays

Can it be done? The accelerator problems are soluble and the top-up frequency is negotiable. In fact it HAS been done:

Turning on SPEAR injection (to clear ions) with feedback orbit control ON Is routine (shutters closed)

Top-up operation of CESR is now routine for high energy physics ; dT= 1 hour
X-ray experimenters can and do leave shutters open

Some CESR experiments collect data during top-up; preliminary scans, alignment, in some instances real data
(e.g. protein crystallography)

Longterm prospects

- Trade lifetime for emittance
- Trade lifetime for undulator gap
- Trade lifetime for ring energy
- Ring designs predicated on top-up

Contributions to beam loss rate

Quantum lifetime: occasional emission of a very energetic photon by synchrotron radiation; Usually measured in years

Touschek scattering: intrabunch scattering, transferring transverse momentum into particle energy error

Touschek loss rate α (positron density) $\frac{1}{E^2}\left(\frac{E}{\Delta E_{max}}\right)^2$

Gas scattering α $PZ^2 \ln\left(\frac{E}{\Delta E_{max}}\right)$

bremsstrahlung α $P\frac{Z^2}{E^2}\left(\frac{\beta}{aperture^2}\right)_{max}$ $<\beta>$

elastic

Summed contributions to lifetime, as listed in CDR:

$$\frac{1}{T} = \frac{1}{T_q} + \frac{1}{T_b} + \frac{1}{T_e} + \frac{1}{T_t}$$

quantum brem. elastic touschek

$$= 0 + \frac{P(nT)}{187\ hr} + \frac{P(nT)}{128} + \frac{I(bunch,\ mA)}{950}$$

For APS with = 100mA, P = 1 nT, I(bunch)= 5mA

T = 54 hours with 10% linear coupling

T= 34 hours with 1% linear coupling

Generally, the vertical aperture is the tightest constriction and thus determines the elastic scattering loss rate.

Suppose we assume that, because we know how to top-up, we can reduce the vertical aperture until the lifetime is about

1 hour

What kind of undulators could be installed?

APS

Period (cm)	Ering (GeV)	Gap (cm)	Ephoton (kev)	K
3.3	7.0	1.0-3.3	3.5-13.5	2.4-0.4
2.3	7.0	1.0-2.0	13.0-19.5	1.1-0.3
2.3	6.5	0.4-1.6	3.1-16.0	3.0-0.4
0.53	7.5	0.35	100.	0.11

- In theory, particle beam lifetimes should be about 1 hr. for apertures ~ 2 mm.

ESRF

Period (cm)	Ering (GeV)	Gap (cm)	Ephoton (kev)	K
2.0	6.0	0.4-1.4	4.5-16.0	2.4-0.4

The effect of small vertical aperture on lifetime may be underestimated due to nonlinear coupling. Particles that have undergone Touschek or bremsstrahlung events might be lost on a vertical aperture.

The APS/ASD accelerator physics group has been studying nonlinear coupling in numerical simulations and in experiments at the SRC, Stoughton, WI.

Small gap undulator R&D program at NSLS

DEVELOPMENTS IN HIGH HEAT LOAD X-RAY OPTICS

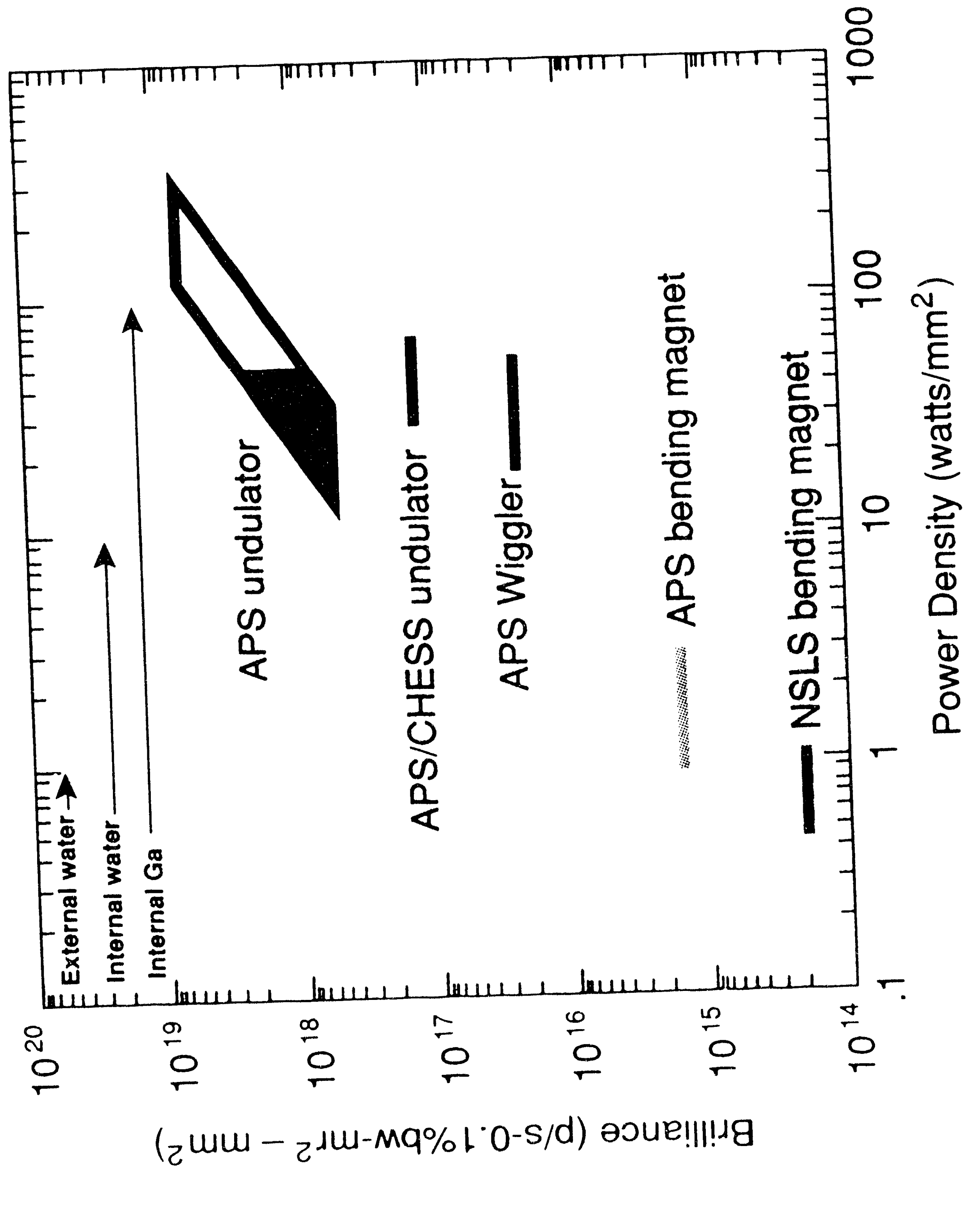
Dennis M. Mills

Fifth Users Meeting
October 13-15, 1992

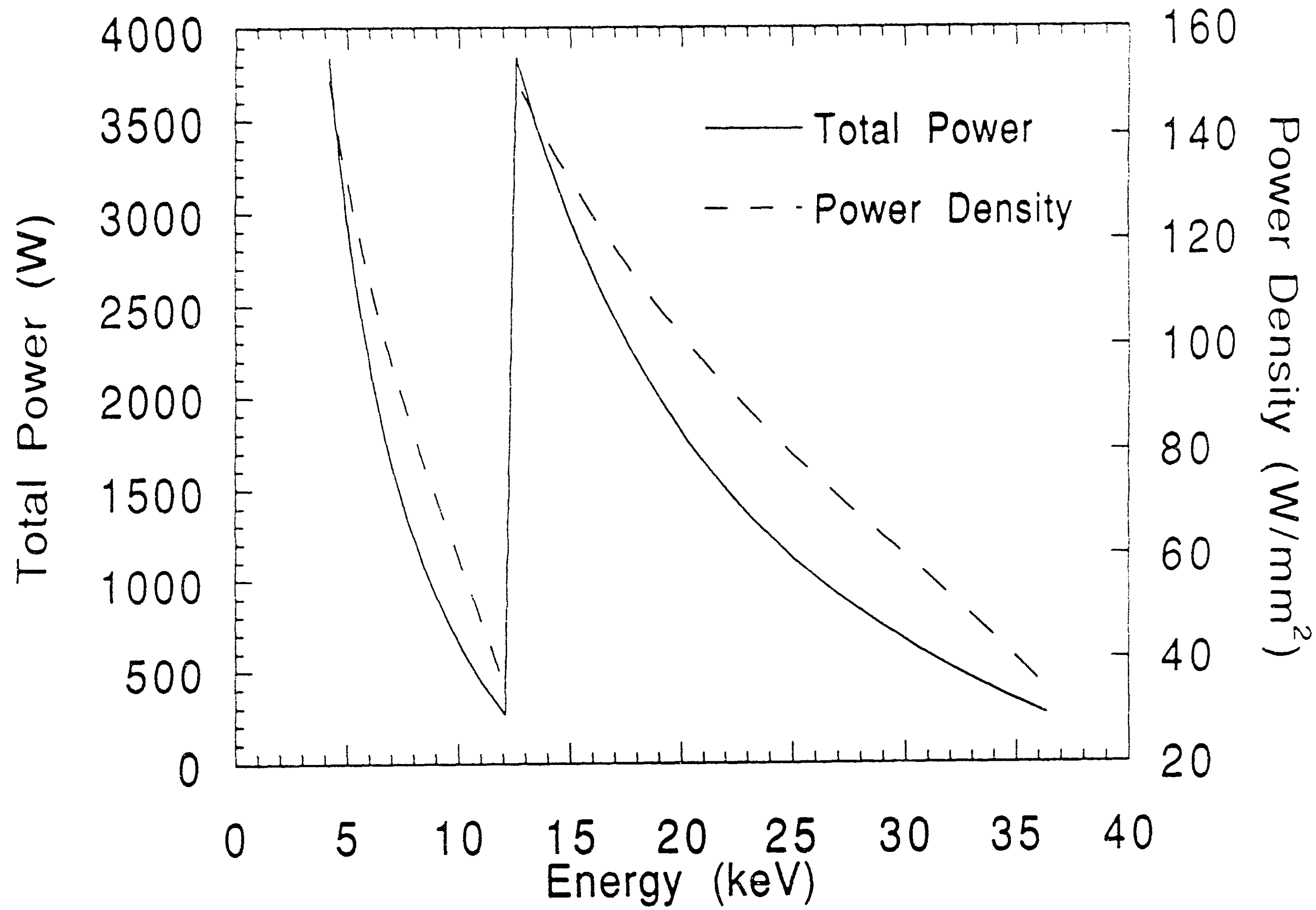
Outline of Presentation

I. INCLINED CRYSTAL WORK
   A. Overview of heat flux spreading
   B. Diffraction properties
   C. Experimental results
   D. Modeling results

II. OTHER ONGOING PROGRAMS
   A. Monochromator procurement
   B. Liquid gallium pump
   C. Pin-post pattern heat exchangers
   D. Modeling efforts
   E. HHL source development
   F. Mirrors as first optical components
   G. Diamond monochromators


External water
Internal water
Internal Ga
APS undulator
APS/CHESS undulator
APS Wiggler
APS bending magnet
NSLS bending magnet
Power Density (watts/mm^2)
Brilliance (p/s-0.1%bw-mr^2 – mm^2)
.1
1
10
100
1000
10^{14}
10^{15}
10^{16}
10^{17}
10^{18}
10^{19}
10^{20}

Undulator A, 3.3 cm period, 30 m from source



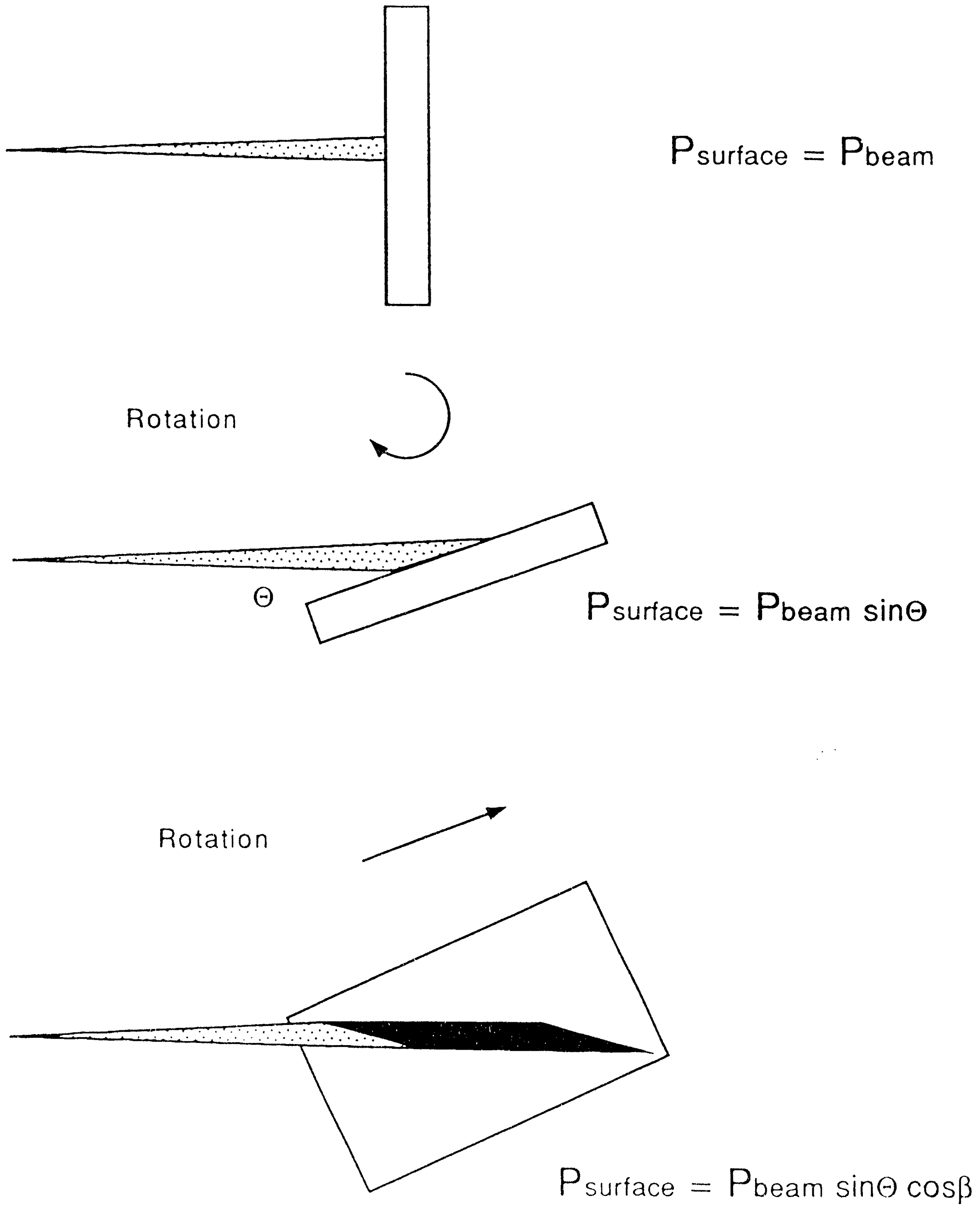
Members of High Heat Load Optics Working Group

Staff:

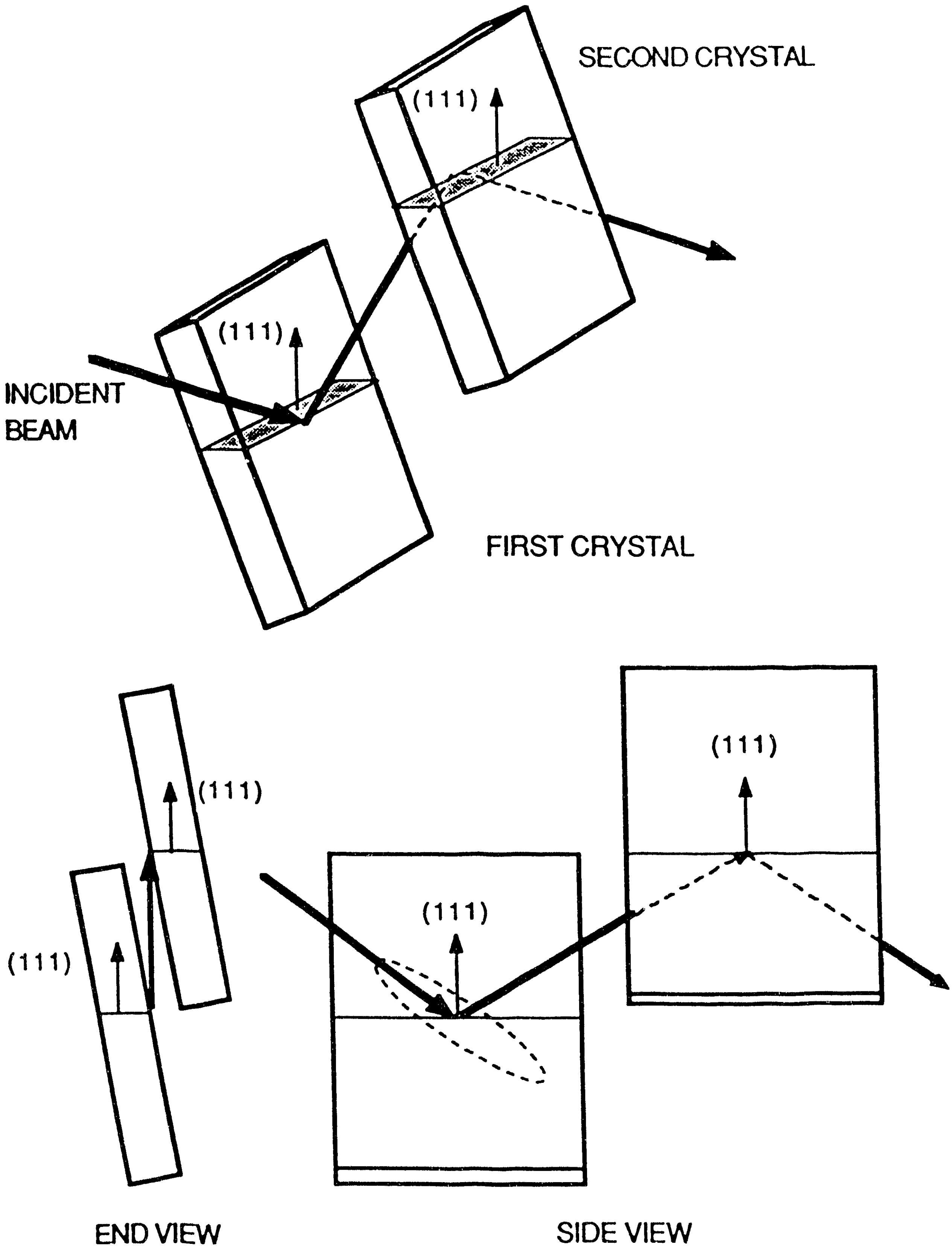
Lahsen Assoufid (8/92)	- analysis and design for focusing mirror for high power density
Steve Davey	- x-ray fabrication lab
Patricia Fernandez	- laser simulation studies
Ali Khounsary*	- FEA modeling, mirrors
Wah Keat Lee	- exp. program, monochromator design, bonding effort
Albert Macrander	- diffraction modeling, exp. program
Dennis Mills	- group leader
Kevin Randall*	- HHL mirrors
Shawn Rogers	- heat transfer, FEA modeling, cryogenic cooling, exp. program
Robert Smither	- liquid gallium pump, exp. program
George Srajer	- specifications for focusing mirror for high power density
Wenbing Yun*	- HHL mirrors
Stefan Joksch (10/92)	- HHL optics program at HASYLAB and with the ESRF
S. Krasnicki (10/92)	- x-ray characterization, HHL experimental program

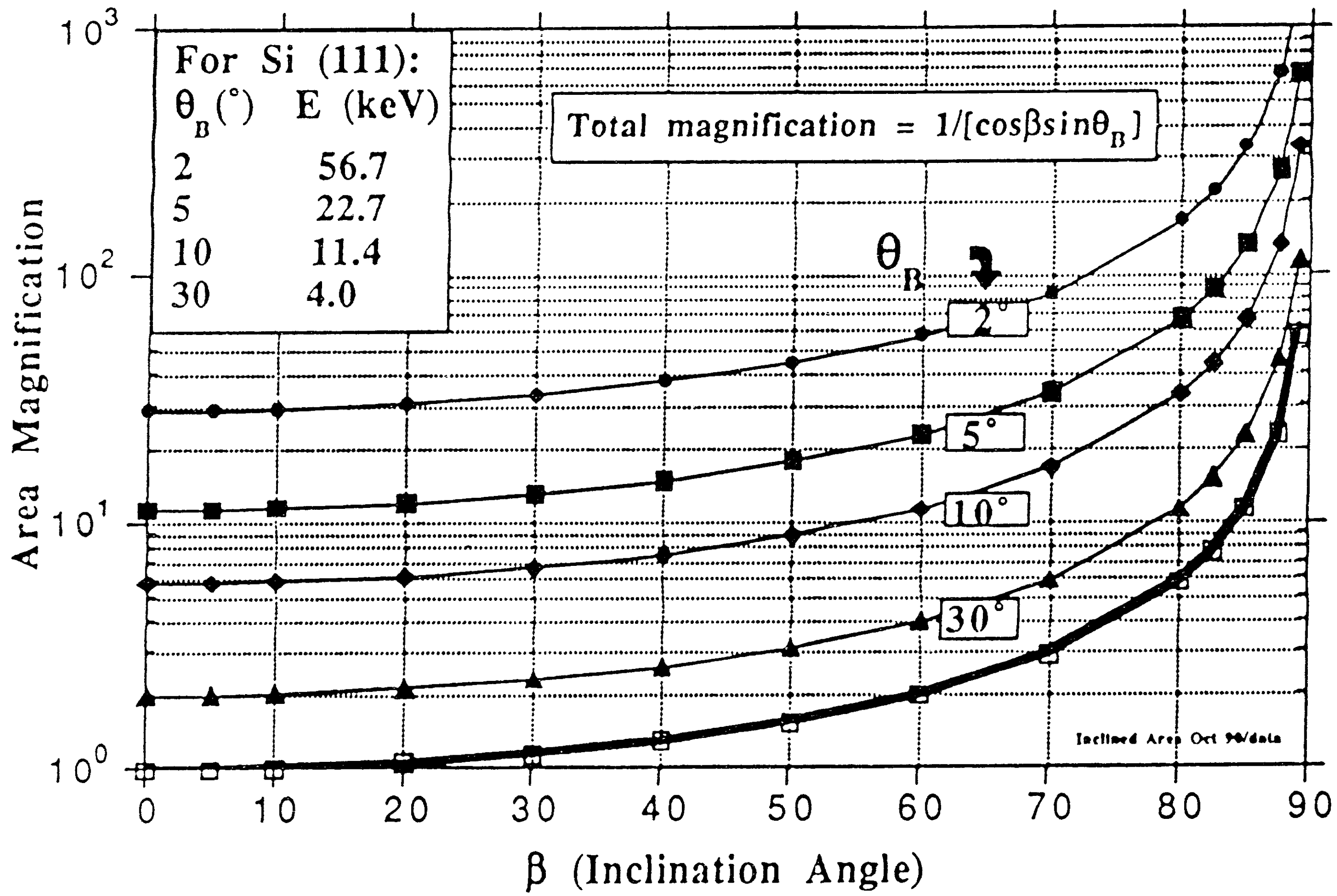
Technicians: Al Paugys, Ron Hopf

* members of another group



$P_{surface} = P_{beam}$
Rotation
Θ
$P_{surface} = P_{beam} \sin\Theta$
Rotation
$P_{surface} = P_{beam} \sin\Theta \cos\beta$


SECOND CRYSTAL
(111)
(111)
INCIDENT
BEAM
FIRST CRYSTAL
(111)
(111)
(111)
(111)
(111)
END VIEW
SIDE VIEW



Magnification of the normal incident beam footprint on an inclined crystal as a function of the inclination angle β for several Bragg angles. Also shown (in heavy line) is the magnification compared to the conventional monochromator footprint as a function of the inlcination angle.

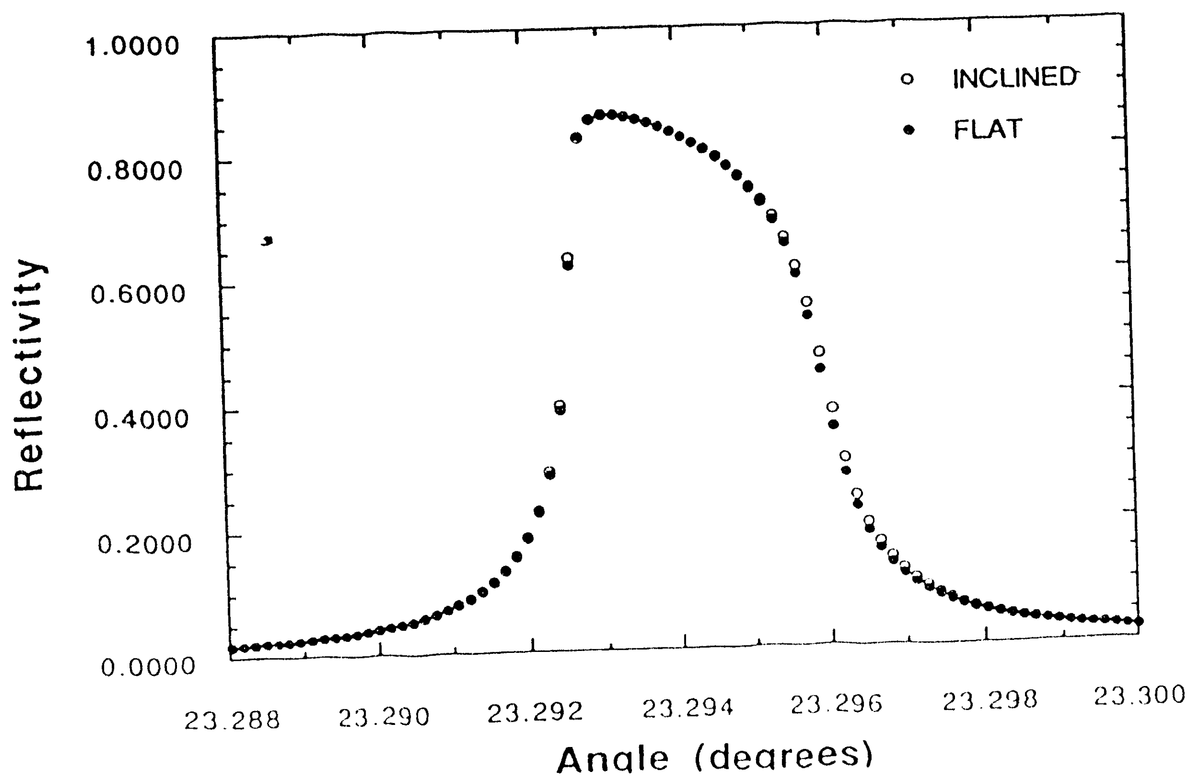
Diffraction Properties of Inclined Crystals

One of the concerns about the inclined crystal geometry was its effect on the x-ray diffraction properties, i.e., was the reflectivity altered from that of the standard or symmetric geometry? No significant differences were found using two independent dynamical diffraction calculations:

- an 8 x 8 matrix calculation (code developed by D. Berreman (AT&T) and A. Macrander (APS)

and

- a 4th order dispersion curve calculation performed by Paul Cowan (ANL).

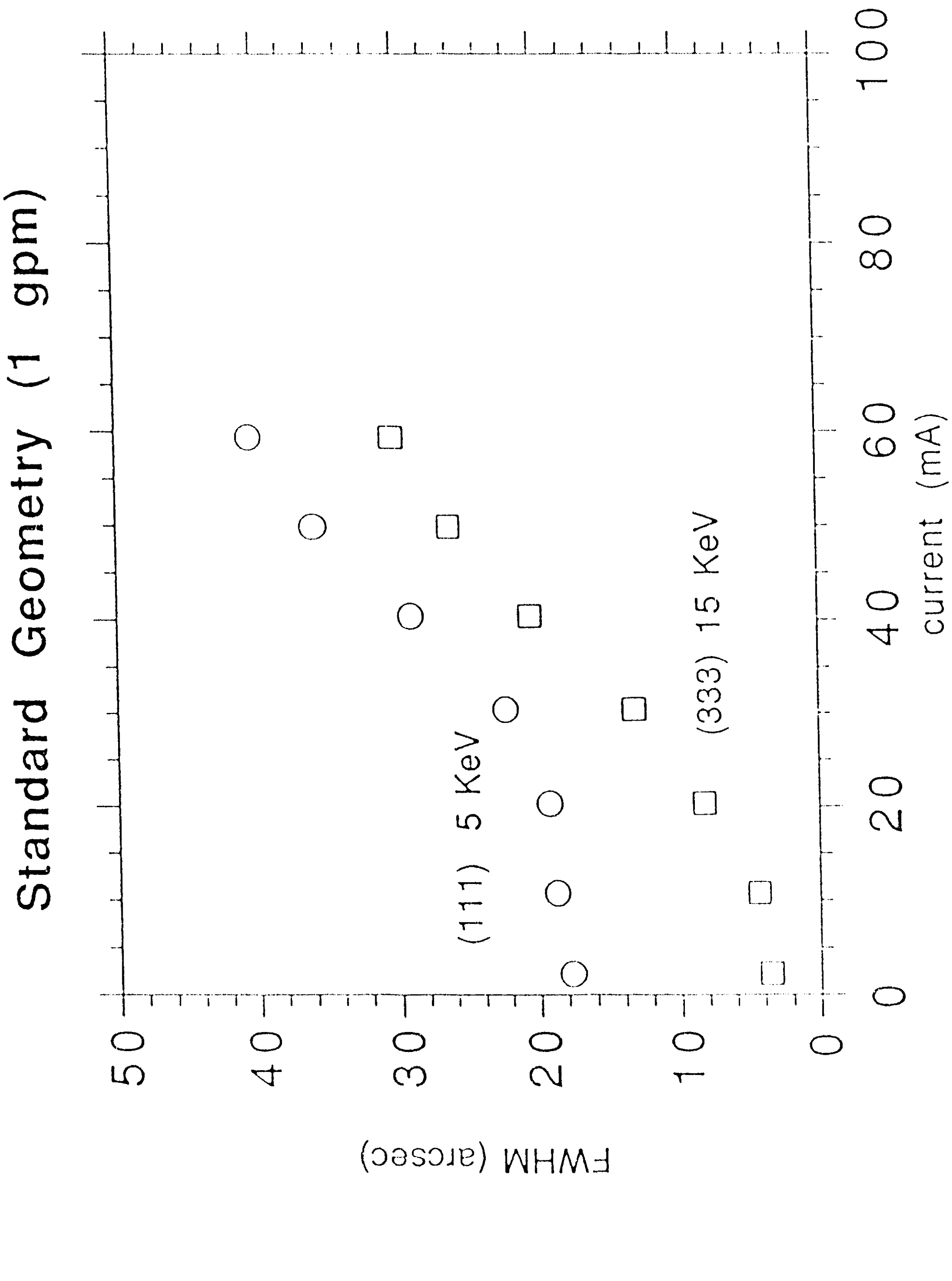


Experimental Results Using the Inclined Crystal

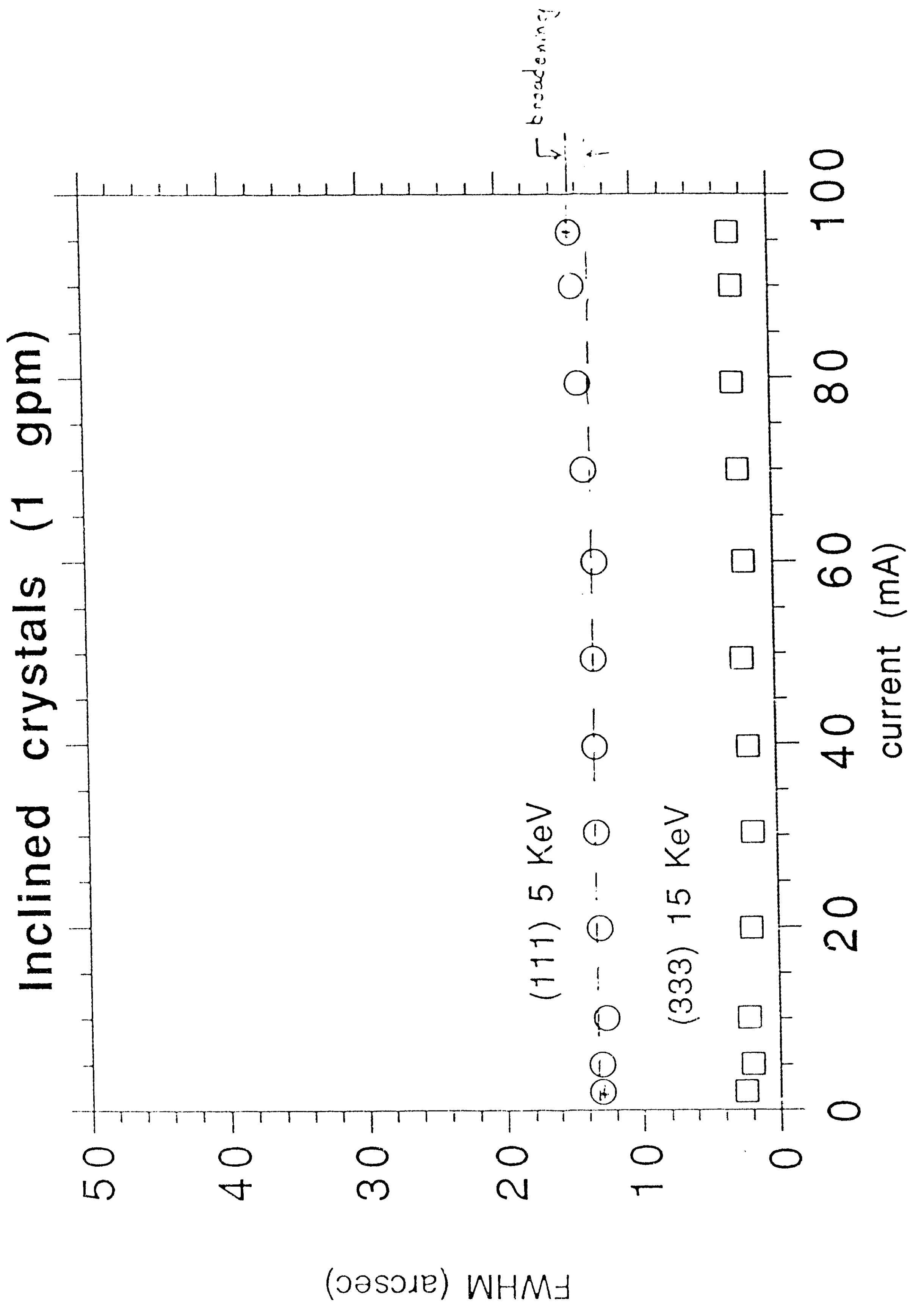
The inclined crystal geometry has been tested under x-ray high heat load conditions at CHESS using the APS/CHESS prototype undulator and at the NSLS on the focused wiggler beamline X-25.

Summary of Results

Source	Power (W)	Flux (W/mm^2)	β (°)	Sur. Flux (W/mm^2)	Result
CHESS	379	48	70.5	6.3	13% loss
NSLS	37.7	118	85	4.1	no loss

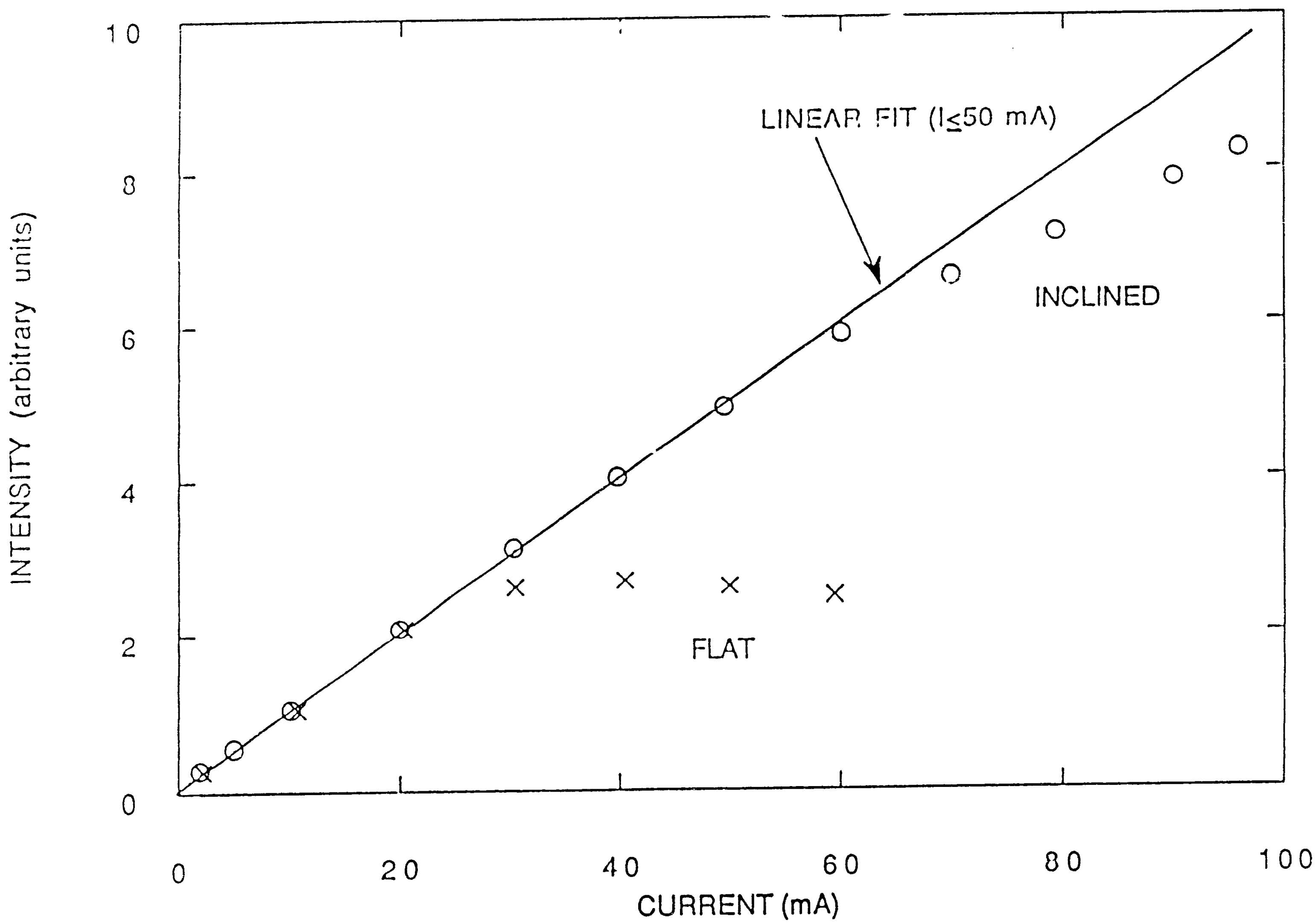


Standard Geometry (1 gpm)
FWHM (arcsec)
50
40
30
20
10
0
0
20
40
60
80
100
current (mA)
(111) 5 KeV
(333) 15 KeV

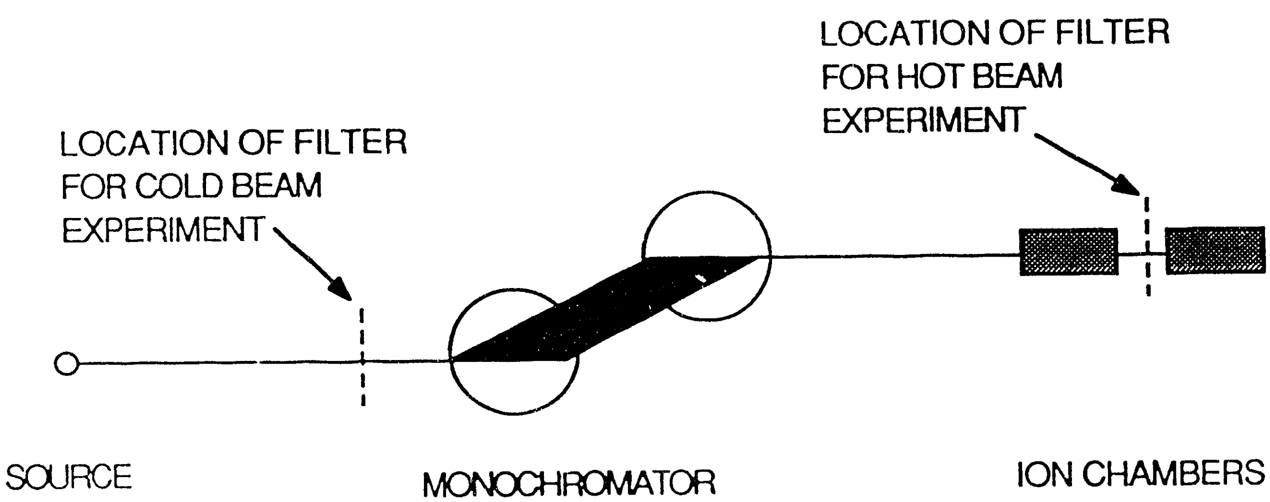


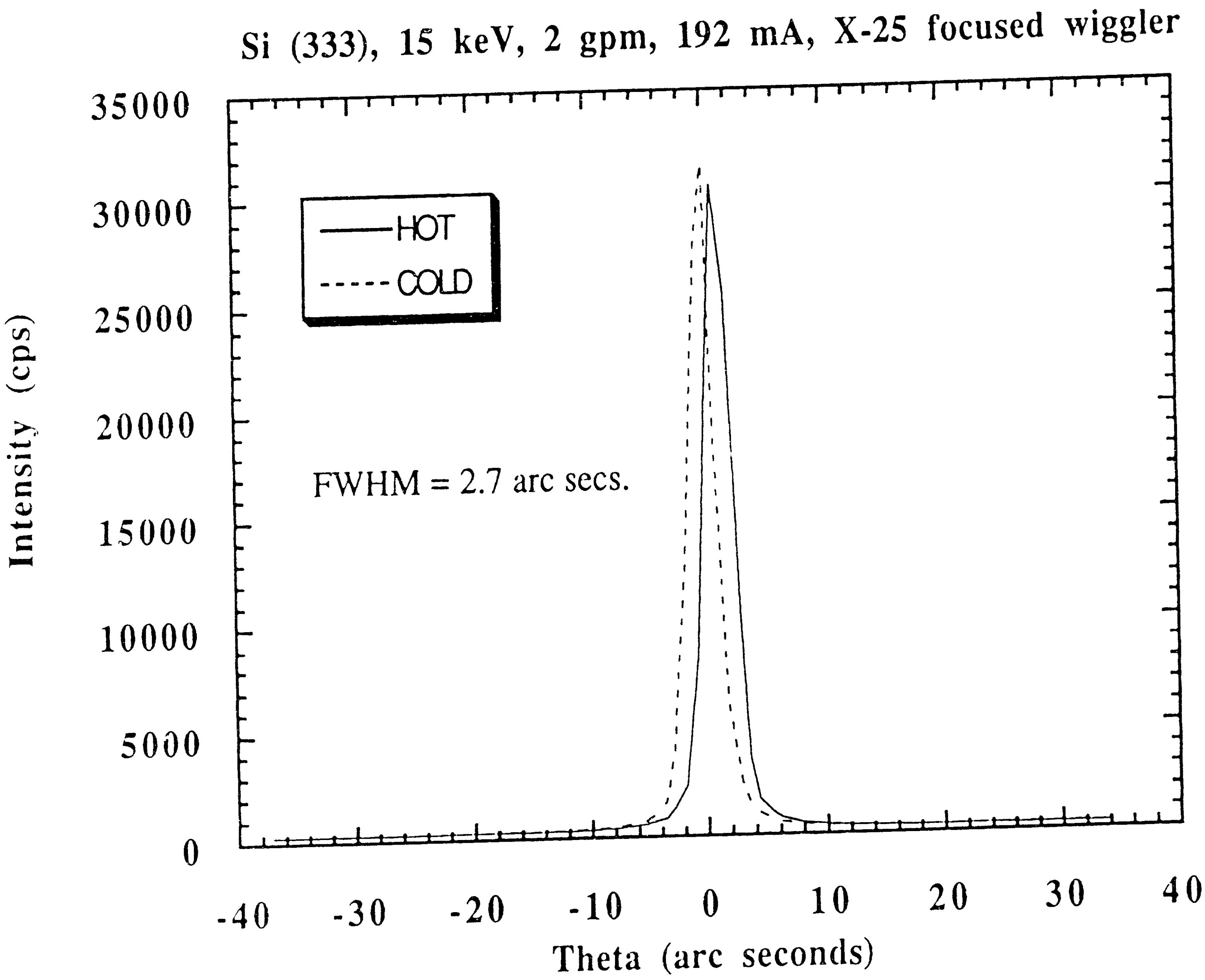
Inclined crystals (1 gpm)
(111) 5 KeV
(333) 15 KeV
broadening
current (mA)
FWHM (arcsec)
0
20
40
60
80
100
0
10
20
30
40
50

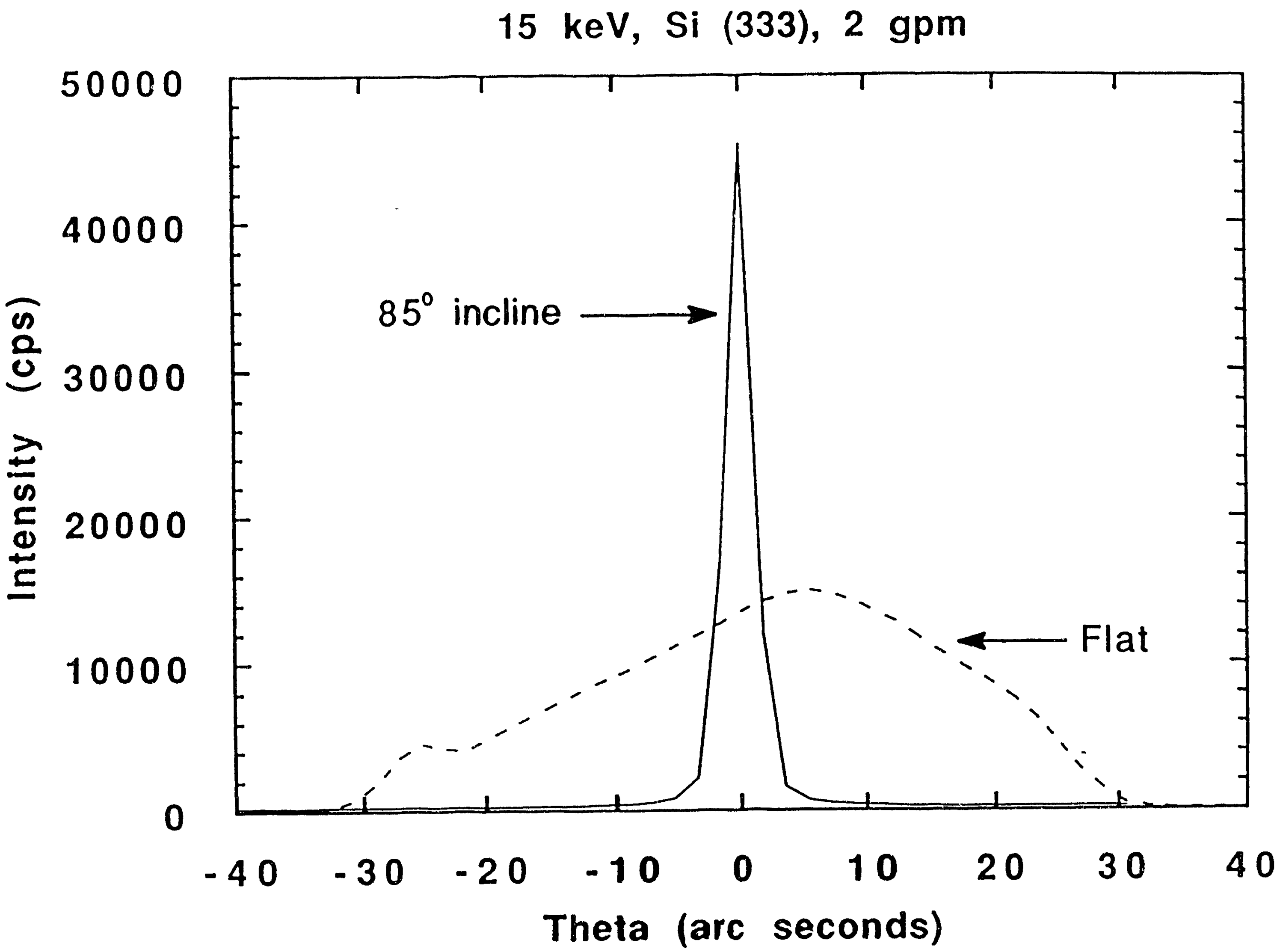
ADVANCED PHOTON SOURCE



ADVANCED PHOTON SOURCE



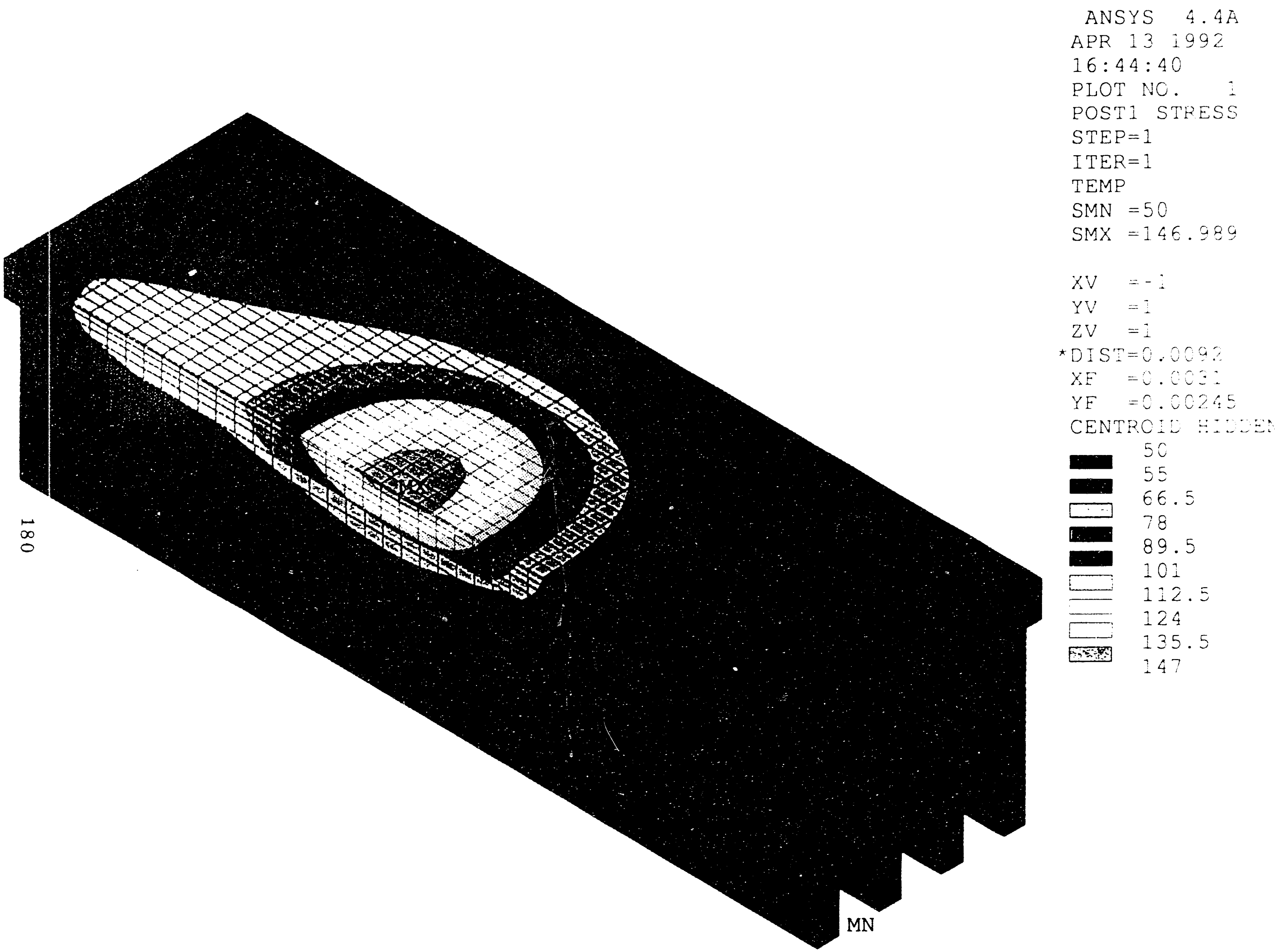

Si (333), 15 keV, 2 gpm, 192 mA, X-25 focused wiggler
35000
30000
25000
20000
15000
10000
5000
0
Intensity (cps)
HOT
COLD
FWHM = 2.7 arc secs.
-40
-30
-20
-10
0
10
20
30
40
Theta (arc seconds)



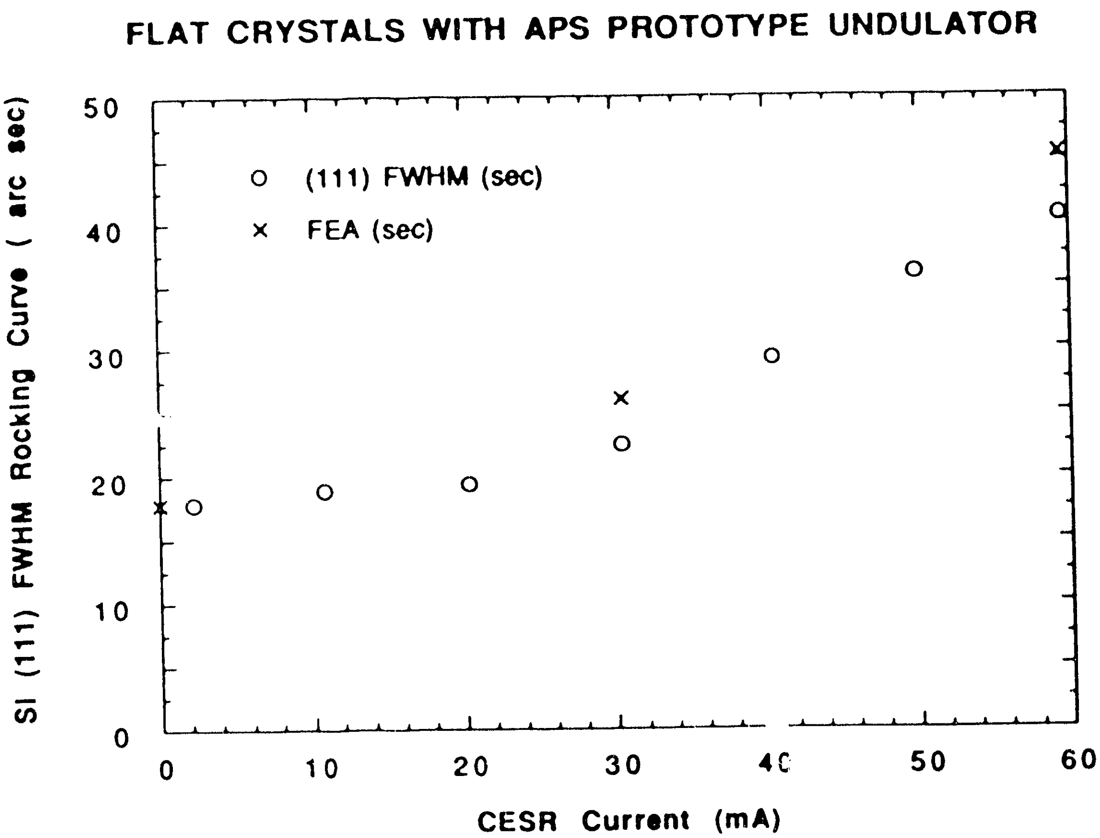
W.K. Lee, A.T. Macrander, D.M. Mills, C.S. Rogers and R.K. Smither, NIM A, 1992, in press.

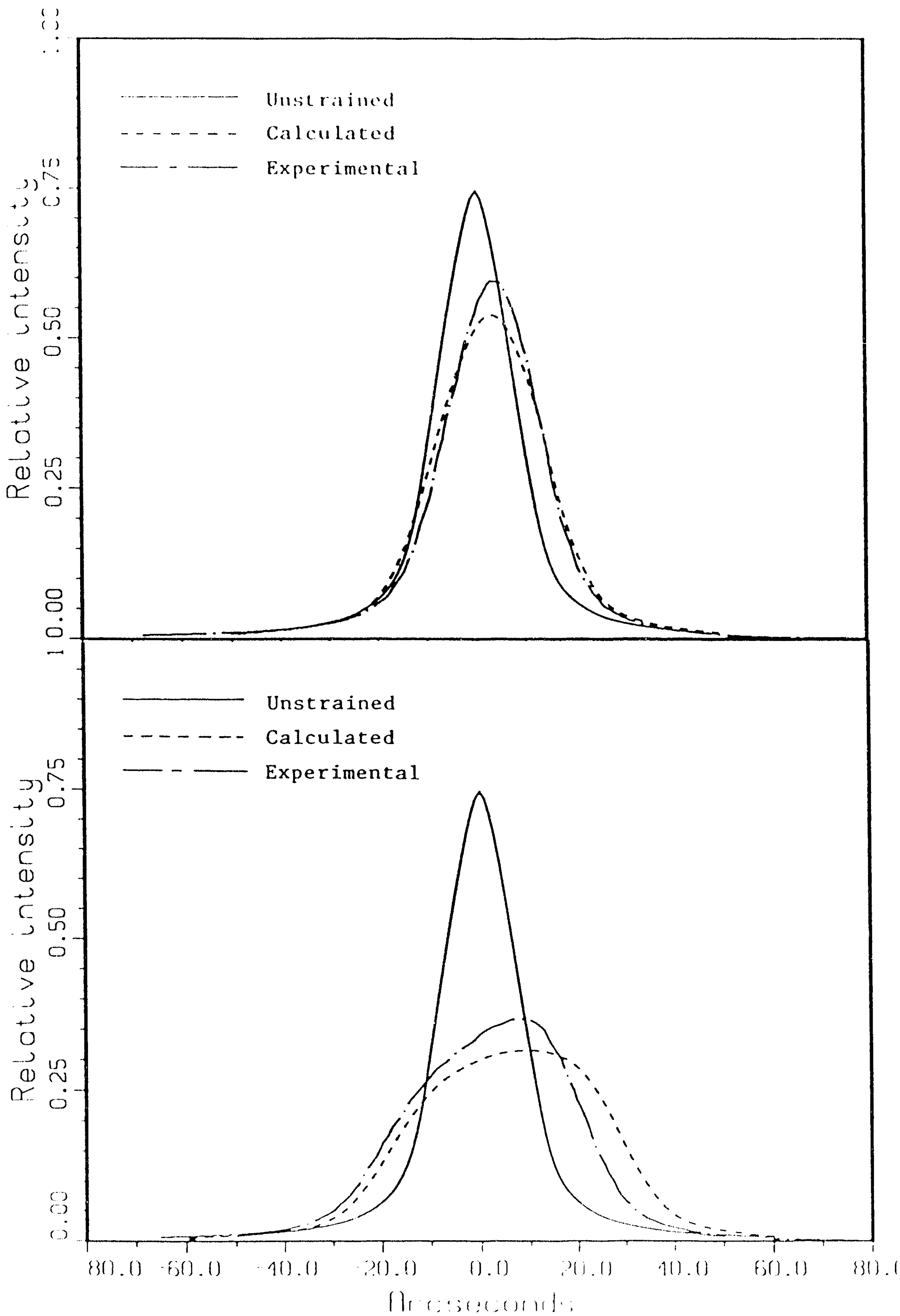
Modeling Results

Both analytical and finite element analysis of the temperature distributions and corresponding distortions of the inclined crystal have been done. These agree well with our experimental results. Prelimenary analysis of the performance of the inclined crystal geometry with Undulator A have been completed. A more refined and realistic analysis of the inclined crystal's preformance with Undulator A will soon be initiated.



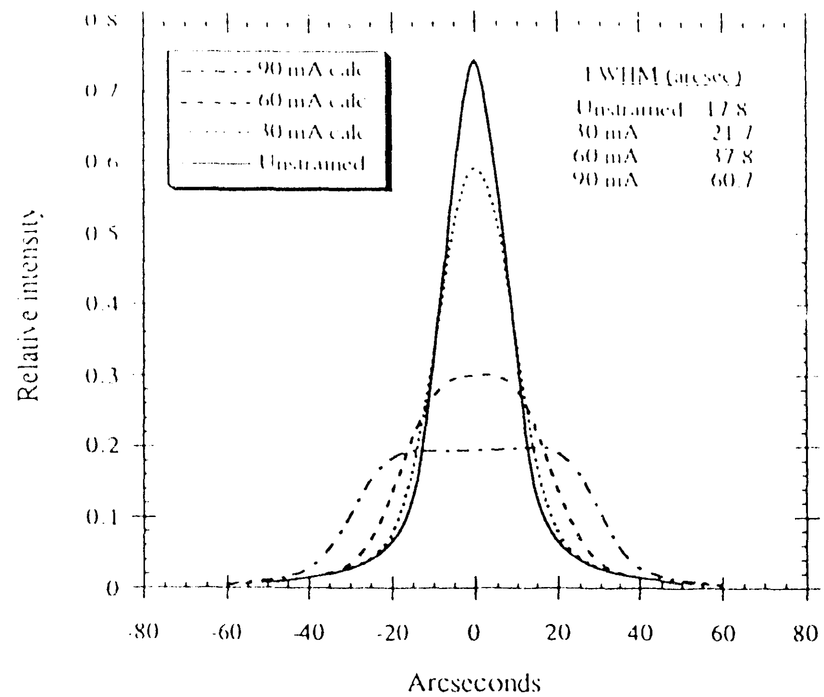
ANSYS 4.4A
APR 13 1992
16:44:40
PLOT NO. 1
POST1 STRESS
STEP=1
ITER=1
TEMP
SMN =50
SMX =146.989
XV =-1
YV =1
ZV =1
*DIST=0.0092
XF =0.0031
YF =0.00245
CENTROID HIDDEN
50
55
66.5
78
89.5
101
112.5
124
135.5
147
MN


FLAT CRYSTALS WITH APS PROTOTYPE UNDULATOR
Si (111) FWHM Rocking Curve (arc sec)
50
40
30
20
10
0
(111) FWHM (sec)
FEA (sec)
0
10
20
30
40
50
60
CESR Current (mA)

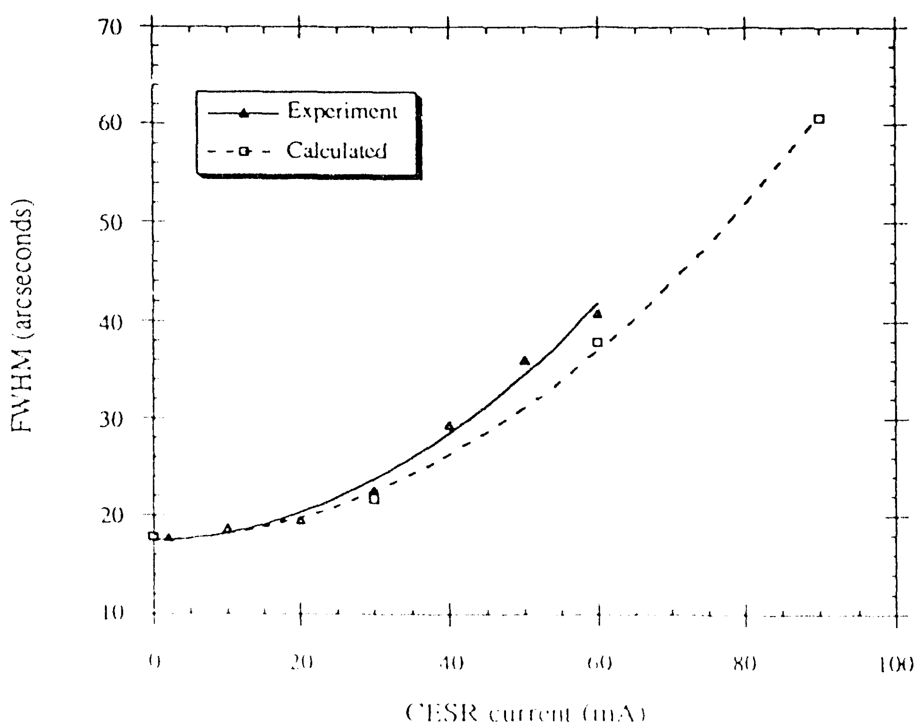


Unstrained
Calculated
Experimental
Relative intensity
0.00
0.25
0.50
0.75
1.00
Unstrained
Calculated
Experimental
Relative intensity
0.00
0.25
0.50
0.75
80.0
-60.0
-40.0
-20.0
0.0
20.0
40.0
60.0
80.0

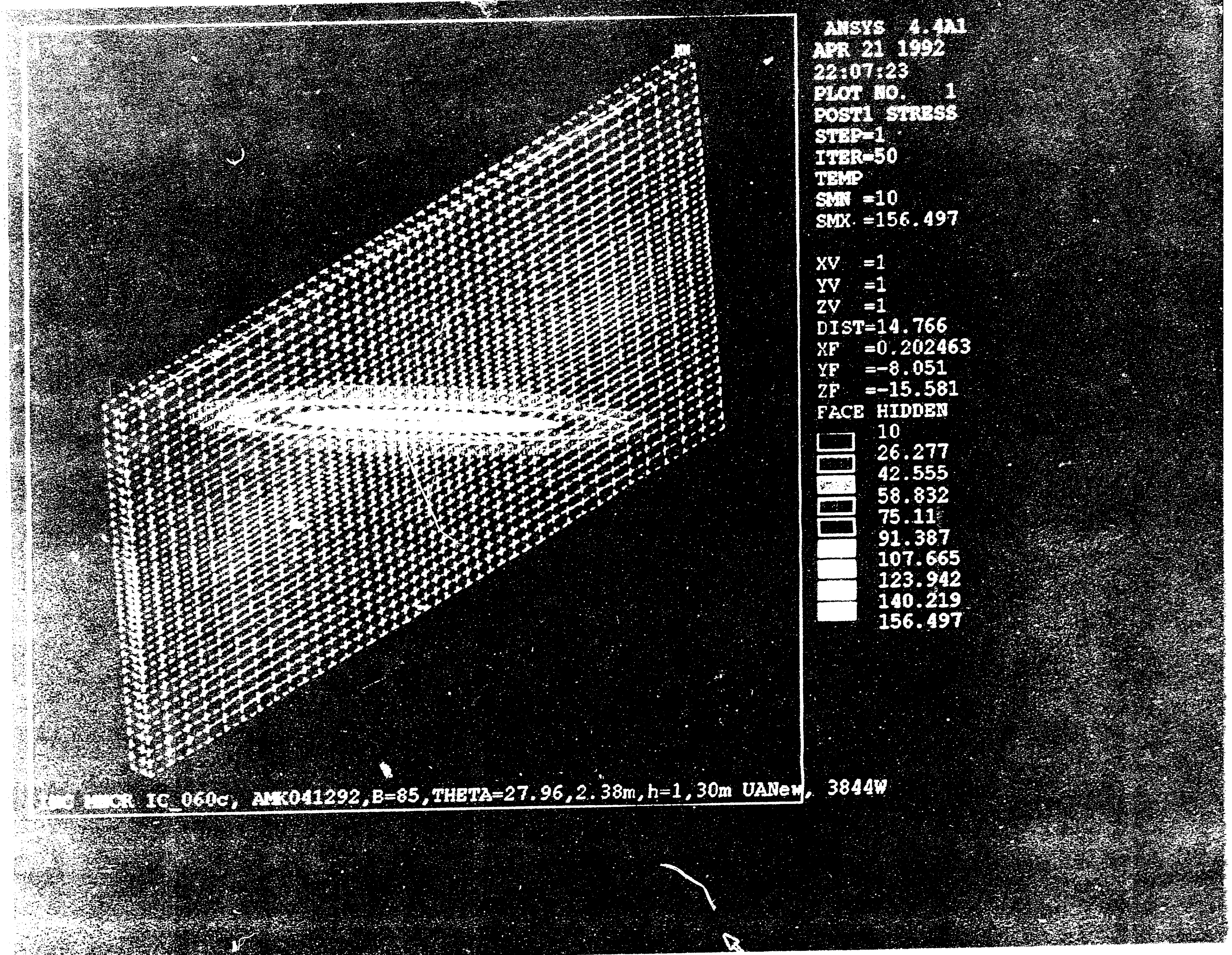
Calculated rocking curves from 2D analytical solution of temperature field for Si(111) double crystal monochromator



Rocking curve full-width at half-maximum intensity



ANSYS Rev.4.4A



Summary of FEA of Inclined Crystal with Undulator A

Case#	K	Slit	Power (kW)	β (°)	Energy (KeV)	Θ (°)	Theory (arcsec)	Cal. (arcsec)	Strain (arcsec)
1	2.2	no	3.8	85	12.6	9.0	6.31	6.52	1.6
2	2.2	yes	0.8	80	12.6	9.0	6.31	8.19	5.2
3	1.5	yes	0.5	80	19.9	5.7	3.94	5.02	3.1
4	1.2	yes	0.4	85	8.2	14.0	10.05	10.24	2.0
5	2.2	yes	0.8	85	4.2	28.0	22.33	22.33	0.0
6 *	2.2	yes	0.8	85	4.2	28.0	22.33	22.75	4.4
7	2.2	no	3.8	85	4.2	28.0	22.33	22.63	3.7

* Case# 6 was identical to Case# 5 except crystal size was larger.

Other Ongoing Programs

- Monochromator Procurement (D. Mills, W. Lee)
  A package for the procurement of the mechanical and vacuum portion of the monochromator has been generated. Vendor proposals are now being evaluated.

- Liquid Gallium Pump (R. Smither)
  A new DC liquid gallium pump has been developed with considerable improvements over the older AC model. That technology has been licensed to a commerical vendor.

- Pin-Post Pattern Heat Exchangers (W. Lee)
  A crystal with an integral pin-post pattern heat exchanger optimized for the APS is being procured.

- Modeling (S. Rogers, A. Khounsary)
  Effort is continuing on the inclined crystal geometry. Analysis of mirrors as first optical components and of cryogenic crystals is being initiated.

- HHL Source Development
  There is a need for higher power and power density sources for testing x-ray optical components than currently exists. Two programs are being pursued:
  - focusing mirror for CHESS wiggler (G. Srajer, L. Assoufid)
  - high power lasers (P. Fernandez)

- Mirrors As First Optical Components (A. Khounsary, K. Randall, W. Yun)
  A program to explore the possibility of using cooled mirrors as first optical components in high heat load beams has been established. Issues to be addressed are thermal distortion of mirror figure, necessity for adaptive optics, and robustness of coatings.

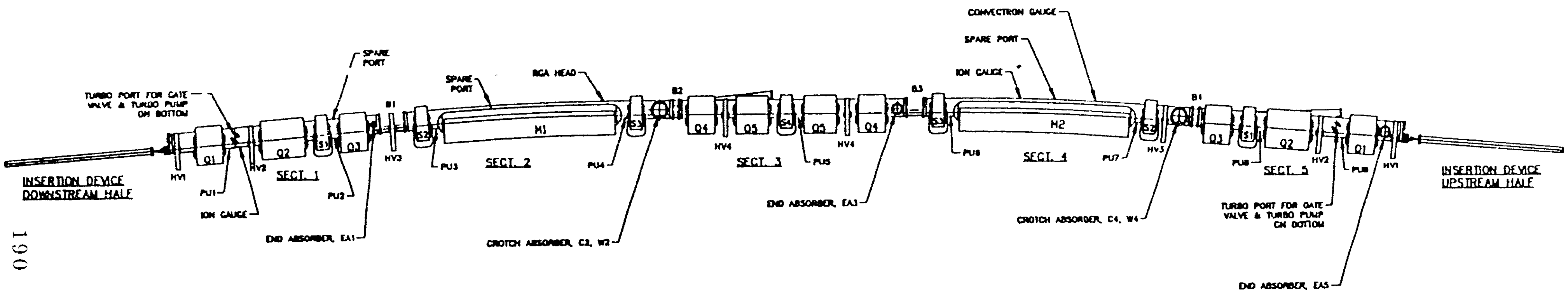
- Diamond Monochromators (S. Davey, A. Khounsary, R. Smither)
  An initital experiment to explore the possible use of diamond crystals as high heat load optical components was completed. This program will be continued with increased vigor in the future.

Strategies for Achieving APS Storage Ring Photon Beam Stability Requirements

Glenn Decker
Storage Ring Manager

ADVANCED PHOTON SOURCE

STORAGE RING LATTICE



S04673
APRIL 22/92

I) Beam Stability Requirements

II) Sources of Beam Motion

A) Mechanical

B) Electrical

III) Remedies

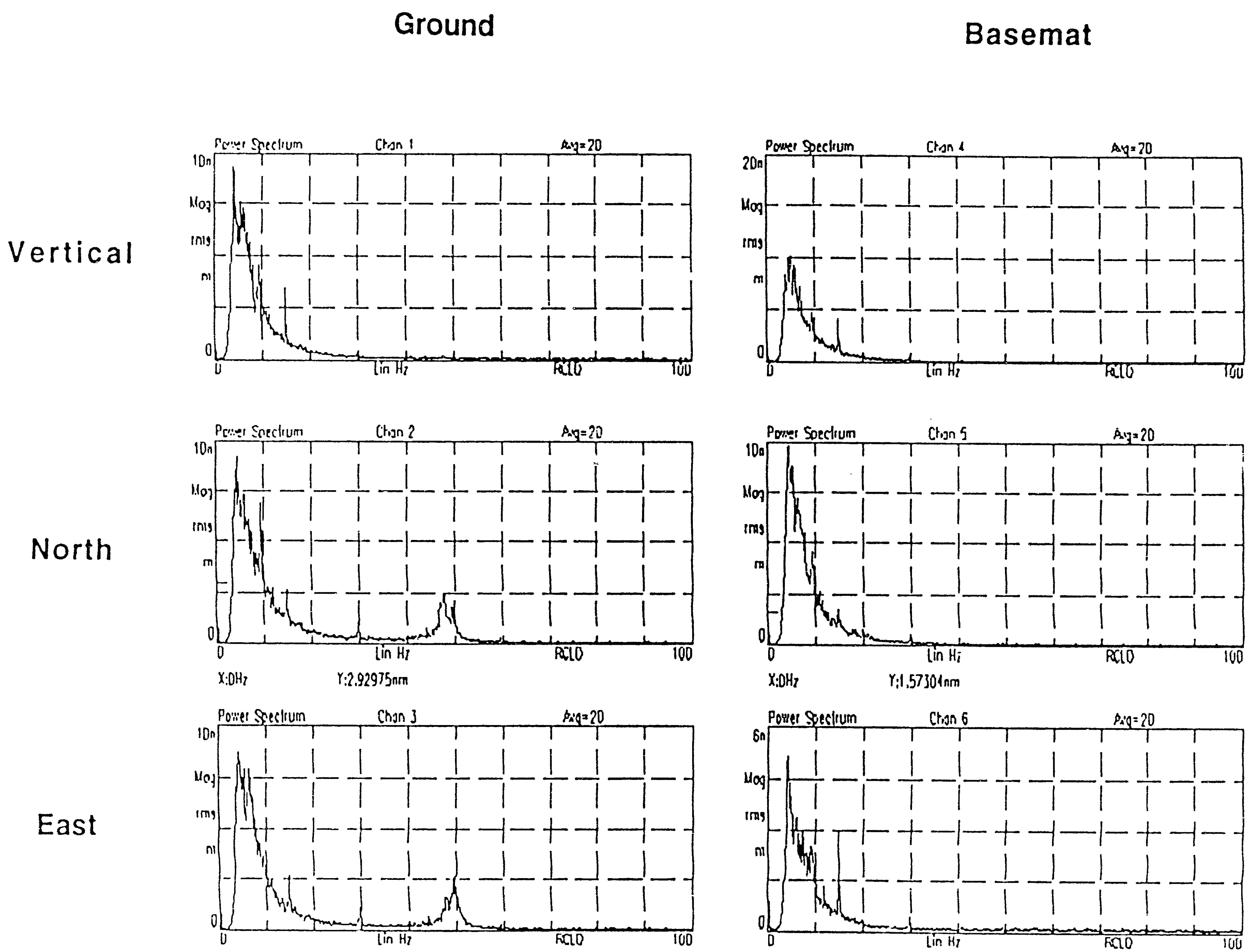
A) Component Specification

B) Design Philosophy

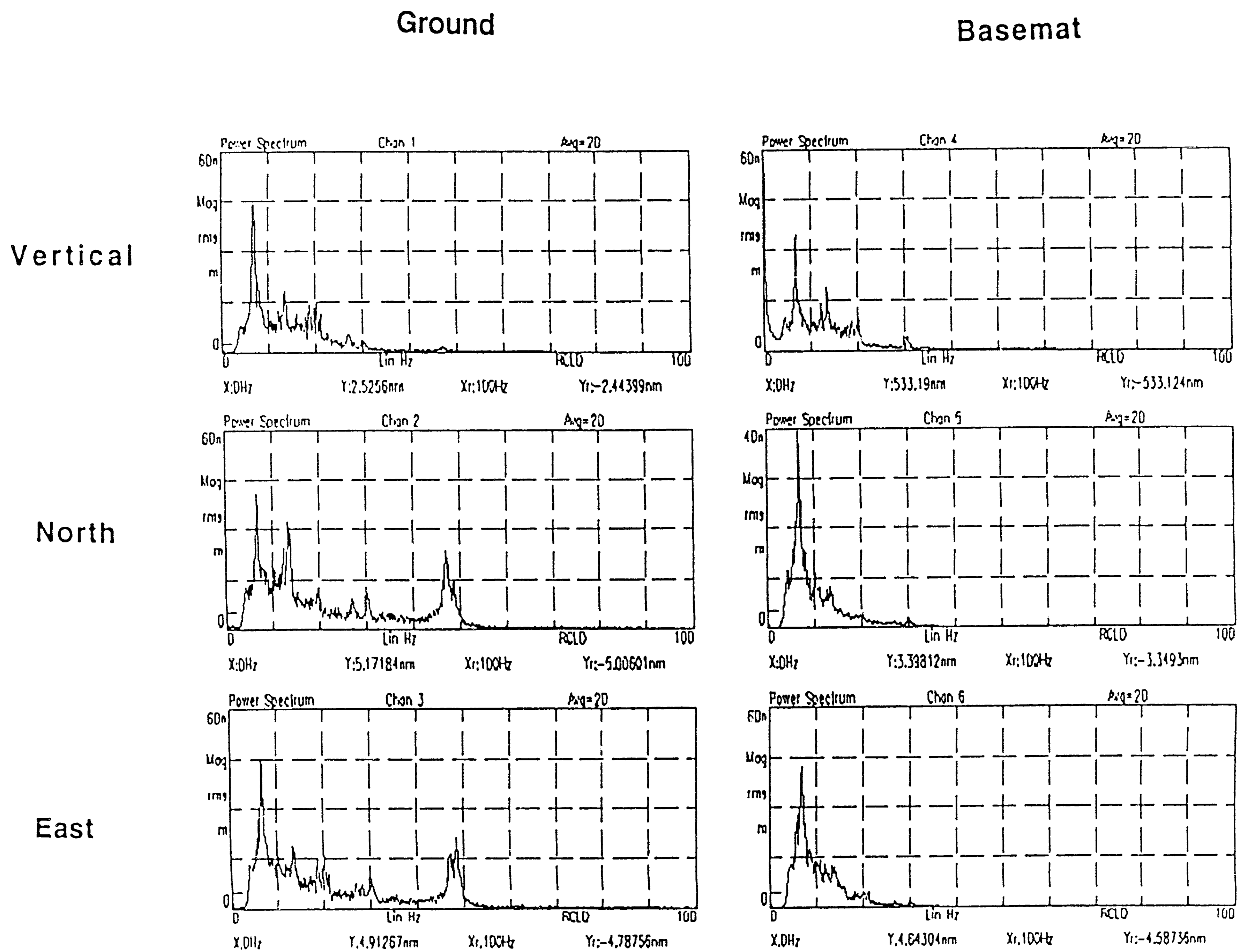
C) Feedback

δ x	δ x'	δ y	δ y'
16 microns	1.2 microrad	4.4 microns	0.45 microrad

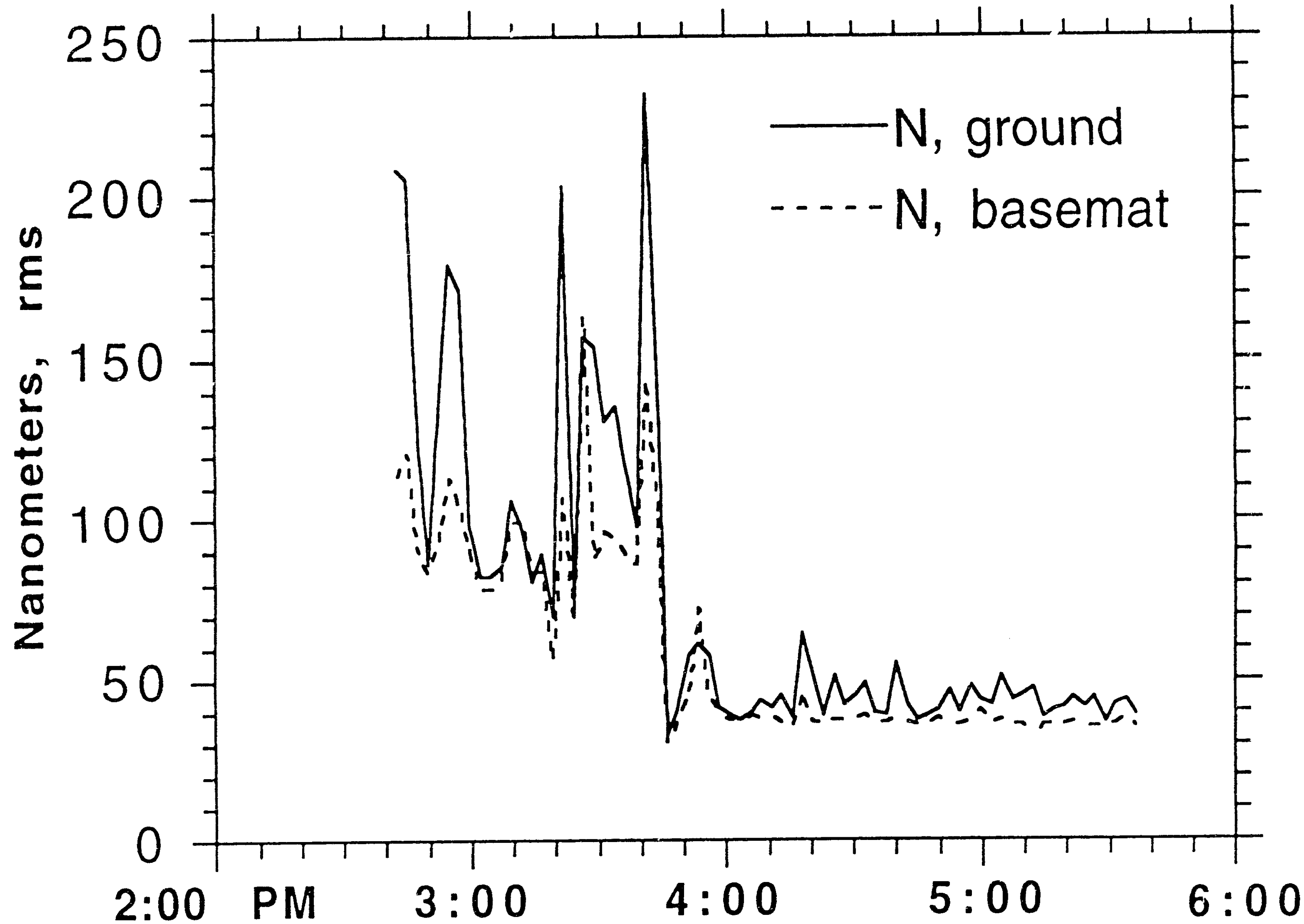
APS Storage Ring Beam Stability Requirements



Typical displacement spectra during quiet period, 5:48 pm



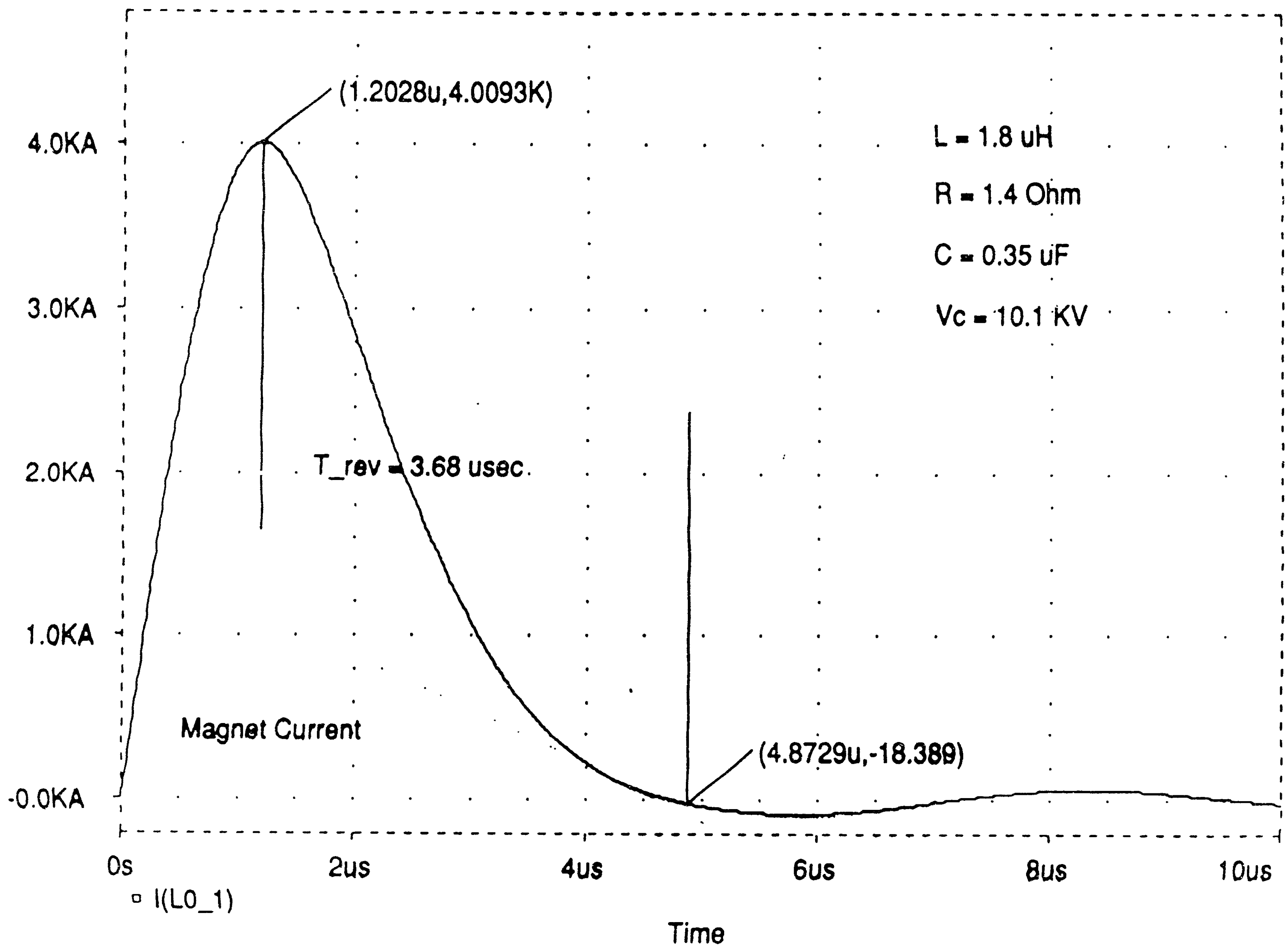
Typical displacement spectra obtained during period of high site activity, 3:24 pm



Ground and basemat displacement, northerly direction, 4-100 Hz

Simulation of Bumper Circuit (B1 On Axis @ 7.7 GeV)

Date/Time run: 06/11/92 11:17:00 Temperature: 27.0



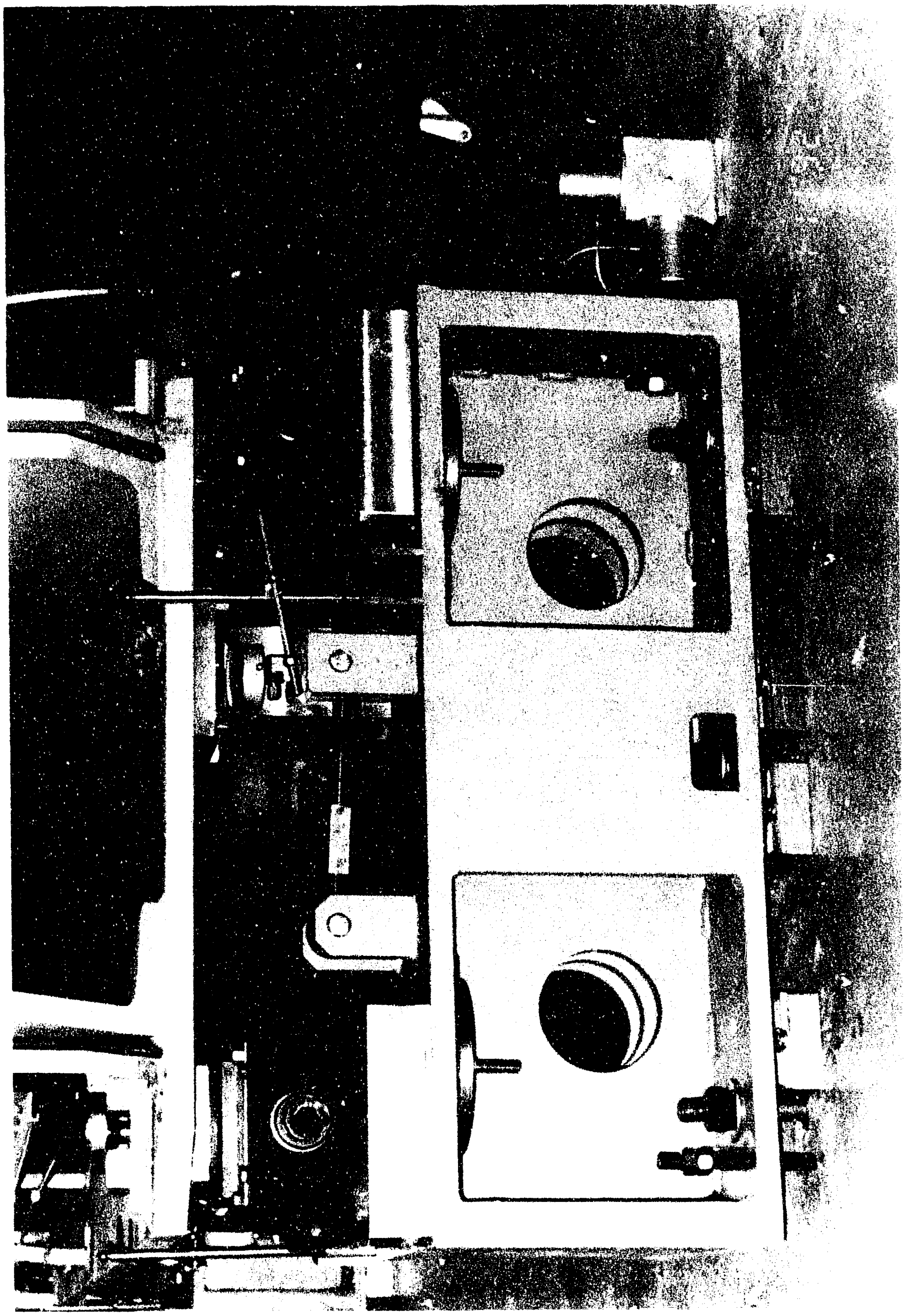
Insertion Device Property	Storage Ring Parameter Affected
Field Integral By dl	Horizontal Beam Position Stability
Field Integral Bx dl	Vertical Beam Position Stability
Second Field Integral By dl dl'	Horizontal Beam Position Stability
Second Field Integral Bx dl dl'	Vertical Beam Position Stability
Quadrupole Integral (d/dx) By dl	Tune, Beam Size
Skew Quadrupole Integral (d/dx) Bx dl	Coupling, Beam Size
Sextupole Integral $(d/dx)^2$ B dl	Dynamic Aperture
Octupole Integral $(d/dx)^3$ B dl	Dynamic Aperture

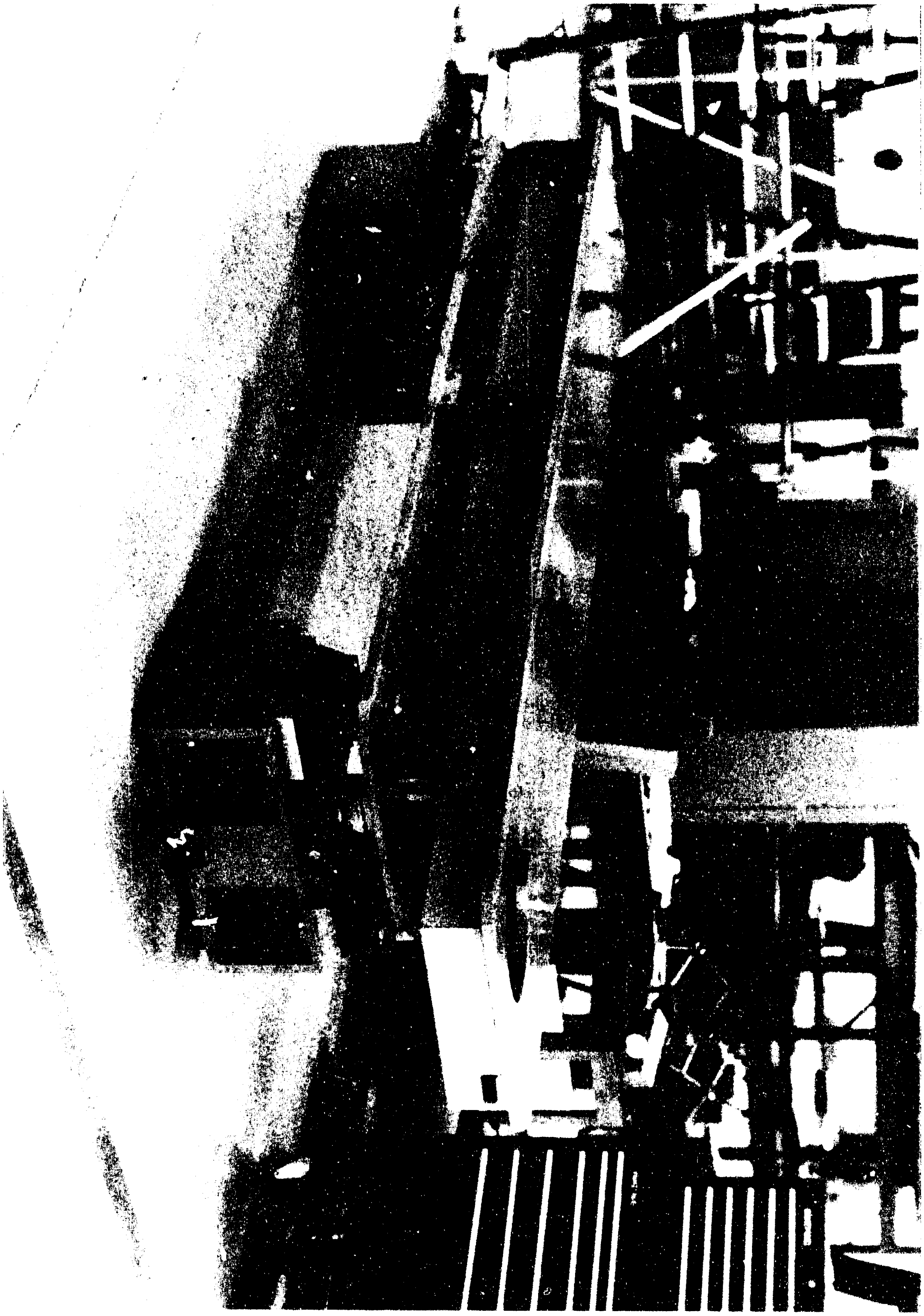
Table 1 Ring Performance Parameters Affected by Insertion Device Field Quality

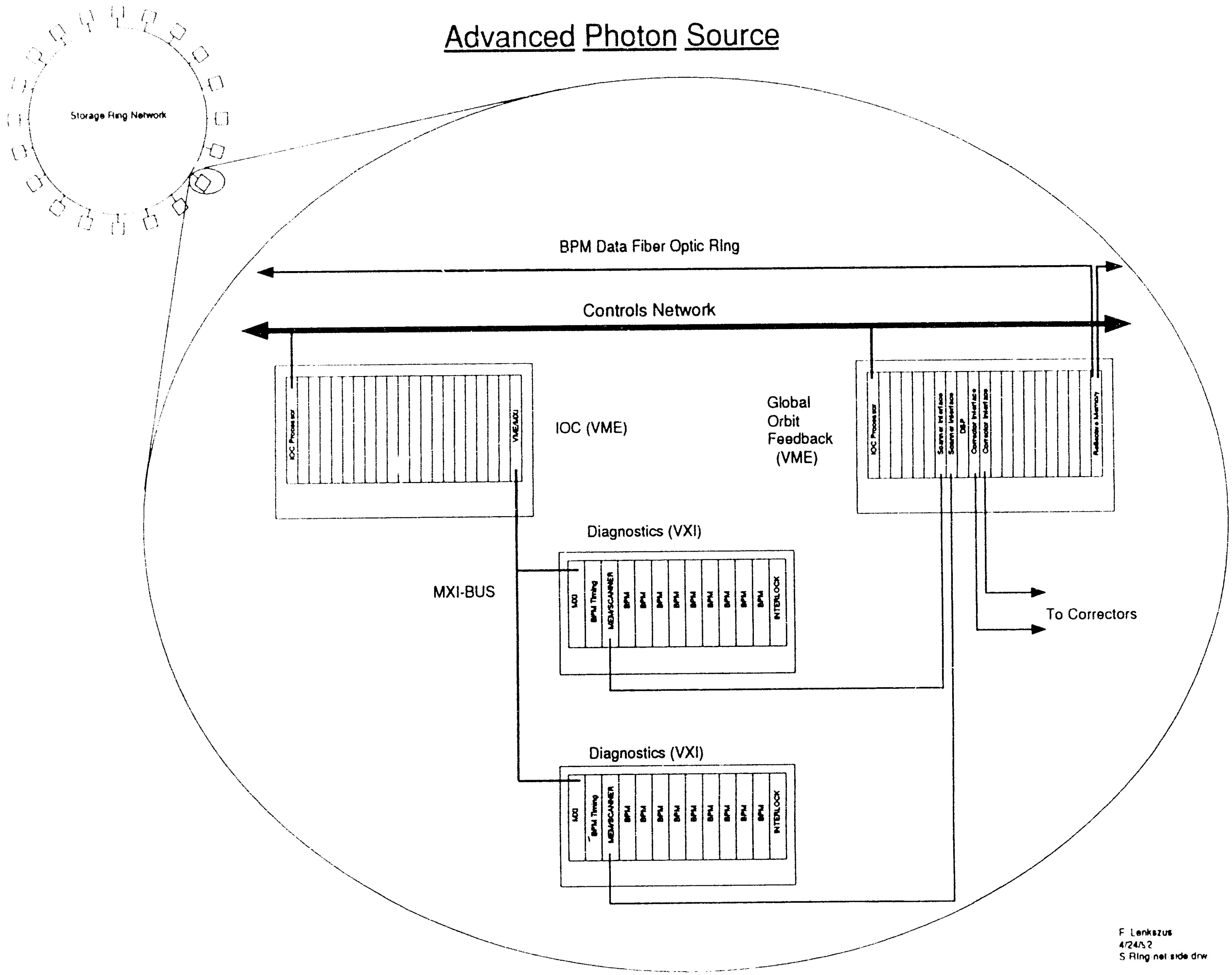
n	Normal Component $B_0 L\ b_n$	Skew Component $B_0 L\ a_n$
0	100 Gauss-cm	100 Gauss-cm
1	50 Gauss	50 Gauss
2	200 Gauss/cm	100 Gauss/cm
3	300 Gauss/cm^2	50 Gauss/cm^2

Table 5 Insertion Device Integrated Multipole Tolerance Specification

$$\int dl\ (B_y + iB_x) = B_0 L \sum_{n=0}^{\infty} (b_n + ia_n) (x + iy)^n$$

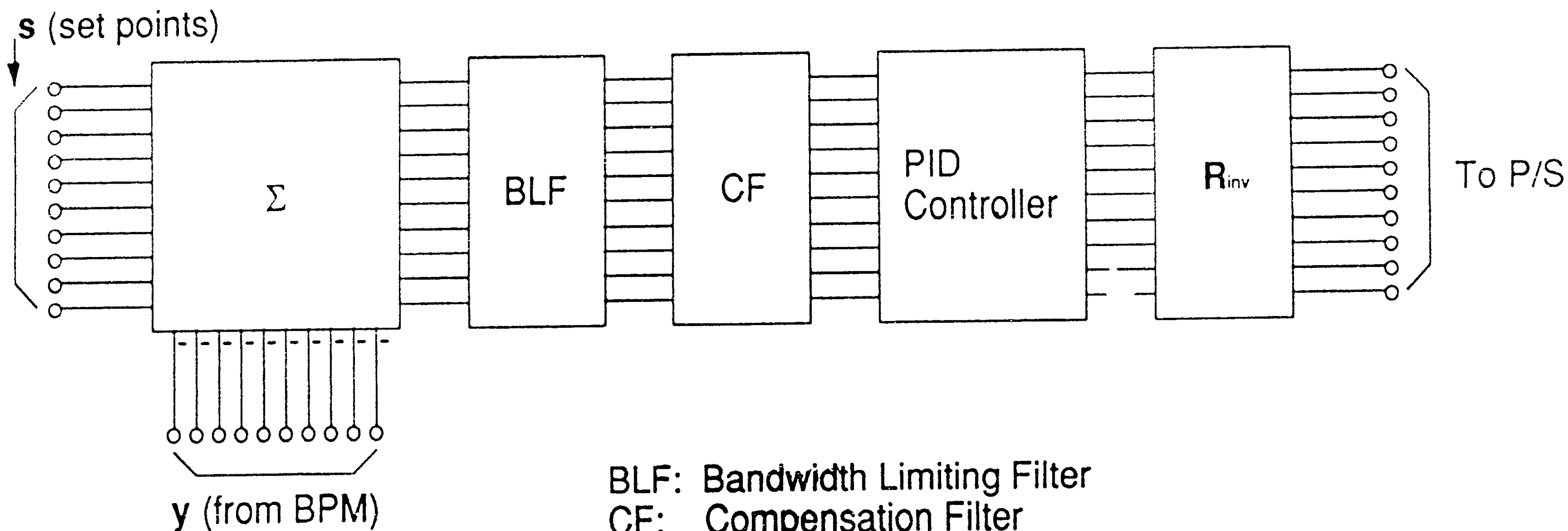






Advanced Photon Source
Storage Ring Network
BPM Data Fiber Optic Ring
Controls Network
IOC Processor
IOC (VME)
Global
Orbit
Feedback
(VME)
Scanner Interface
Scanner Interface
DSP
Corrector Interface
Corrector Interface
Reflective Memory
Diagnostics (VXI)
MXI-BUS
BPM Timing
MEM/SCANNER
BPM
INTERLOCK
Diagnostics (VXI)
To Correctors
F Lenkszus
S Ring net side drw

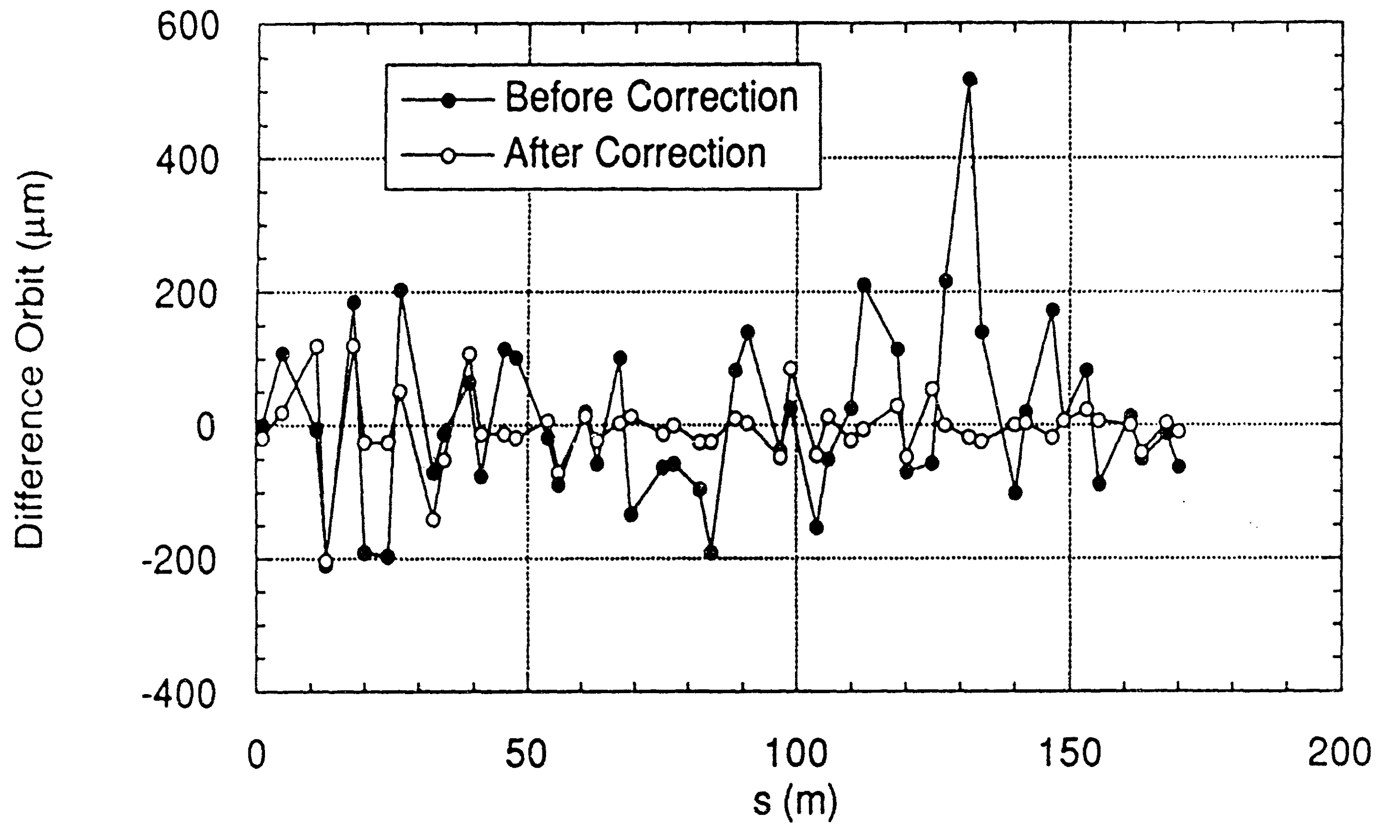
Schematic of AC Global Orbit Correction System for APS Storage Ring



BLF: Bandwidth Limiting Filter
CF: Compensation Filter
P/S: Corrector Magnet Power Supply
BPM: Beam Position Monitor

Schematic of the fast AC global orbit correction system using digital signal processing (DSP) for eddy current compensation, singular value decomposition (SVD) for response matrix inversion ($\mathbf{R}_{inv}$), and proportional–integral–derivative (PID) control algorithm.

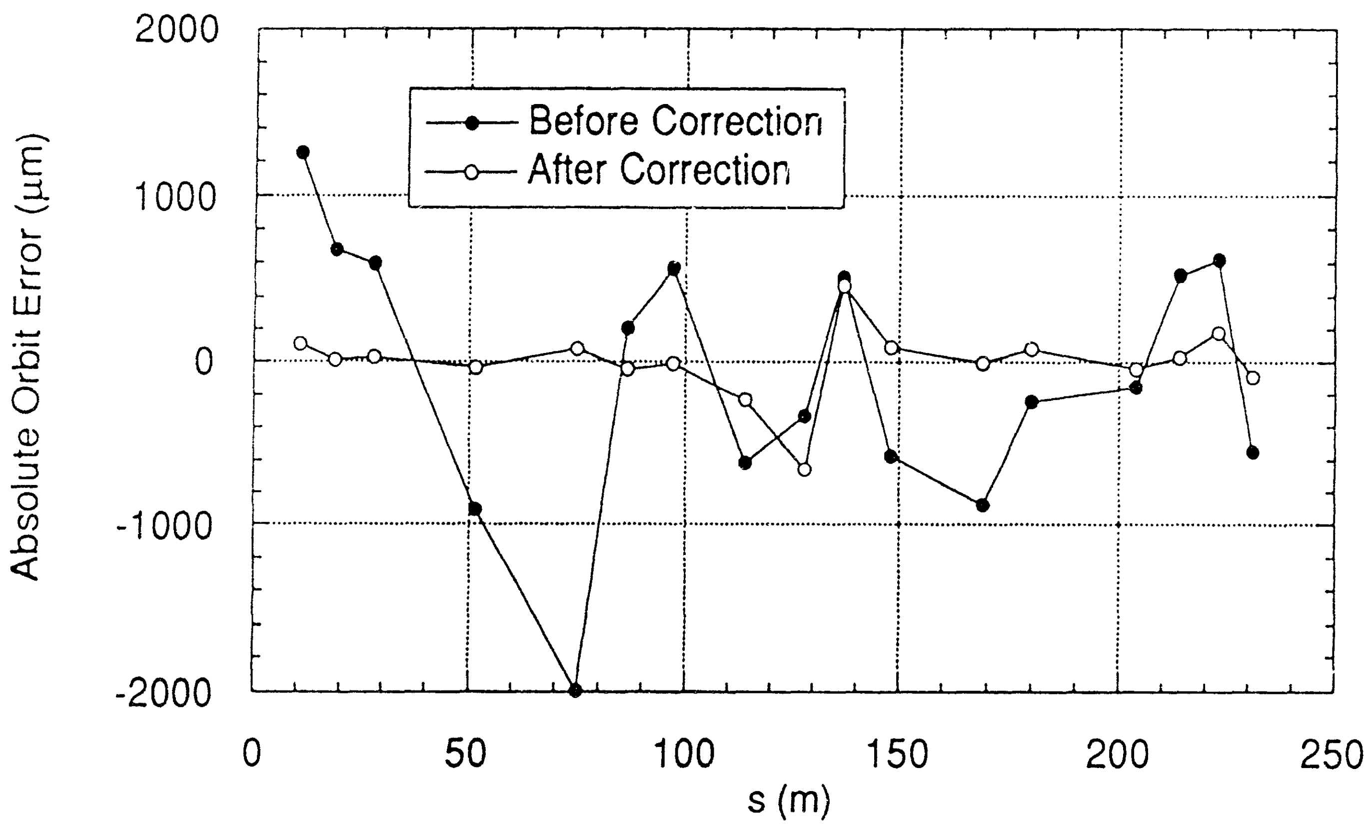
NSLS X-ray Ring Orbit Error Reduced Significantly by DC Global Correction Using SVD Technique (June, 1992)



DC Global orbit correction at NSLS X-ray Ring using the algorithm of singular value decomposition (SVD). The r.m.s. orbit error relative to the reference orbit is 137 μm and 61 μm before and after correction, respectively. (Collaboration with J. Safranek, I. So, and Y. Tang, NSLS).

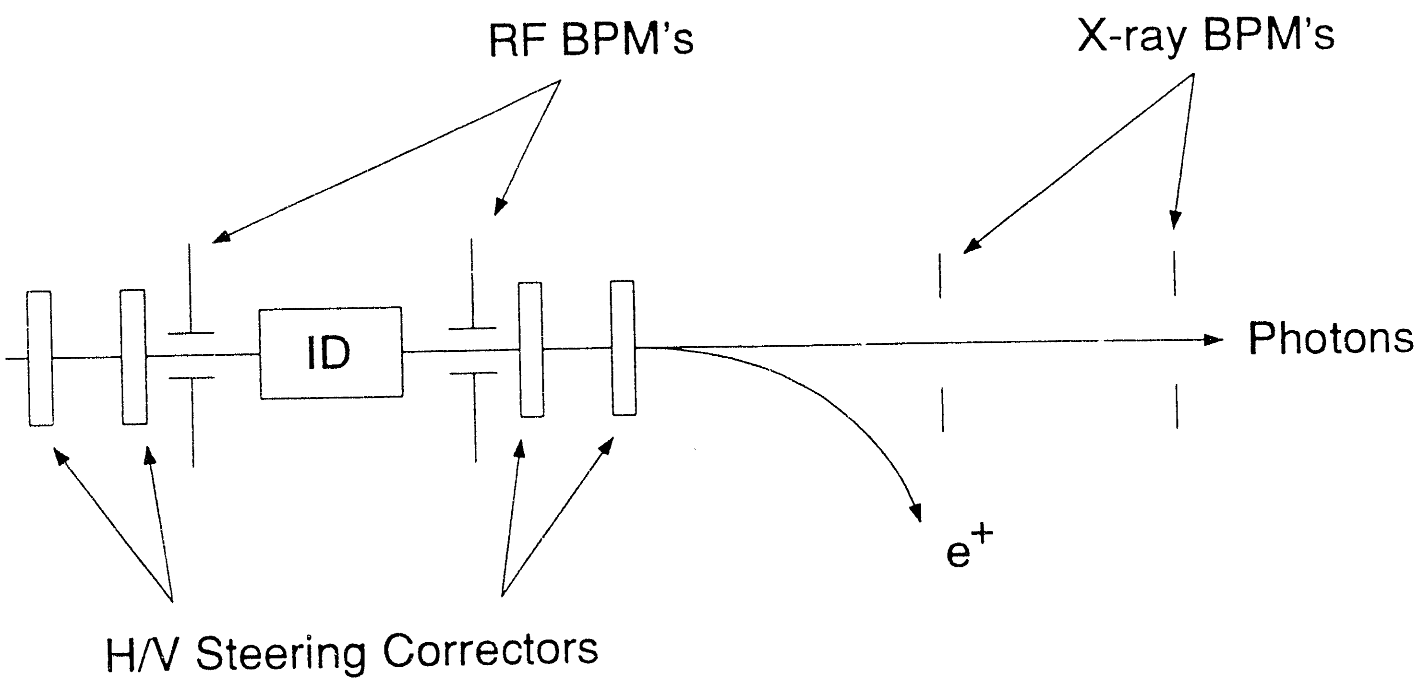
SSRL SPEAR Orbit Error Reduced Dramatically by

DC Global Correction Using SVD Technique (September, 1992)

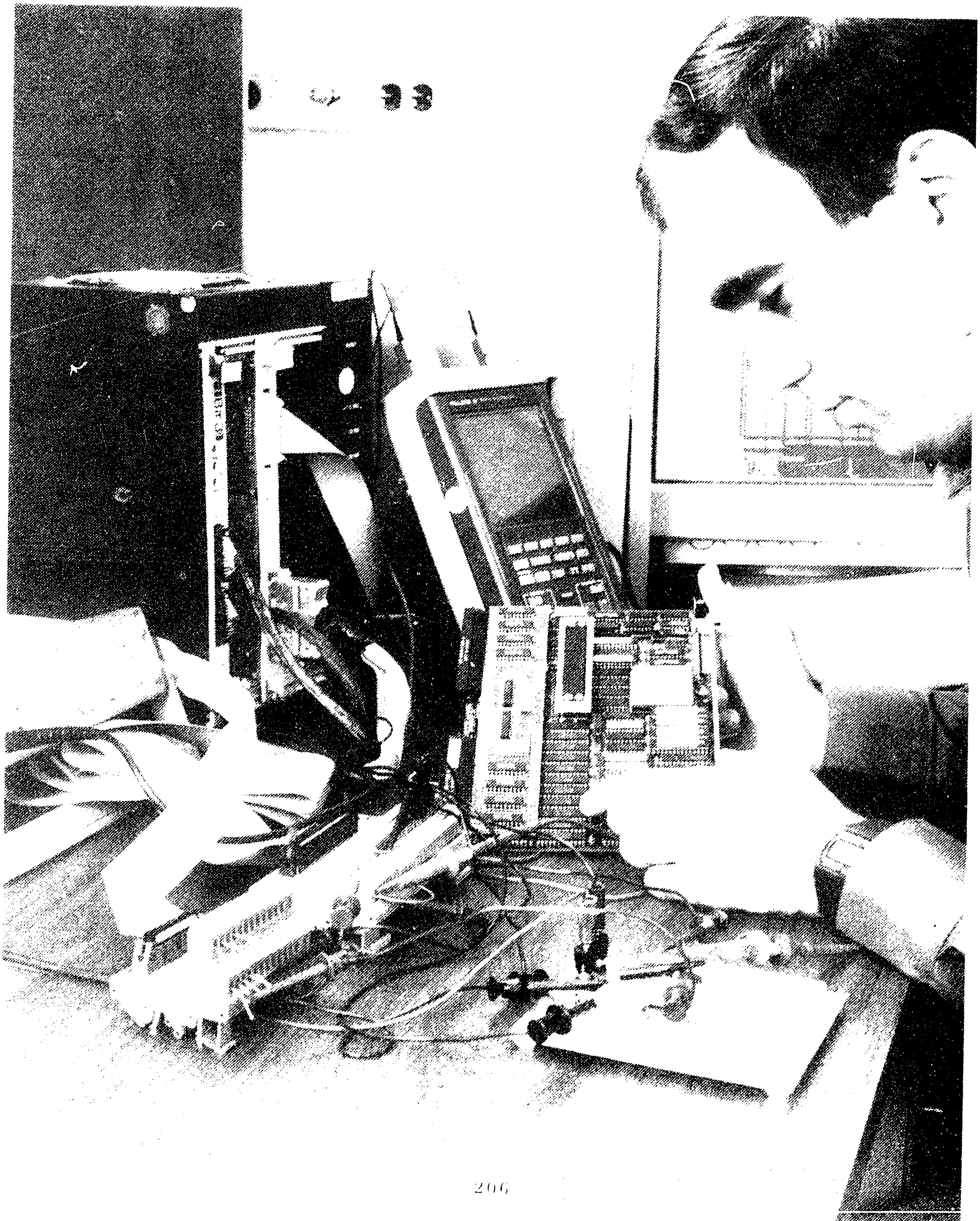


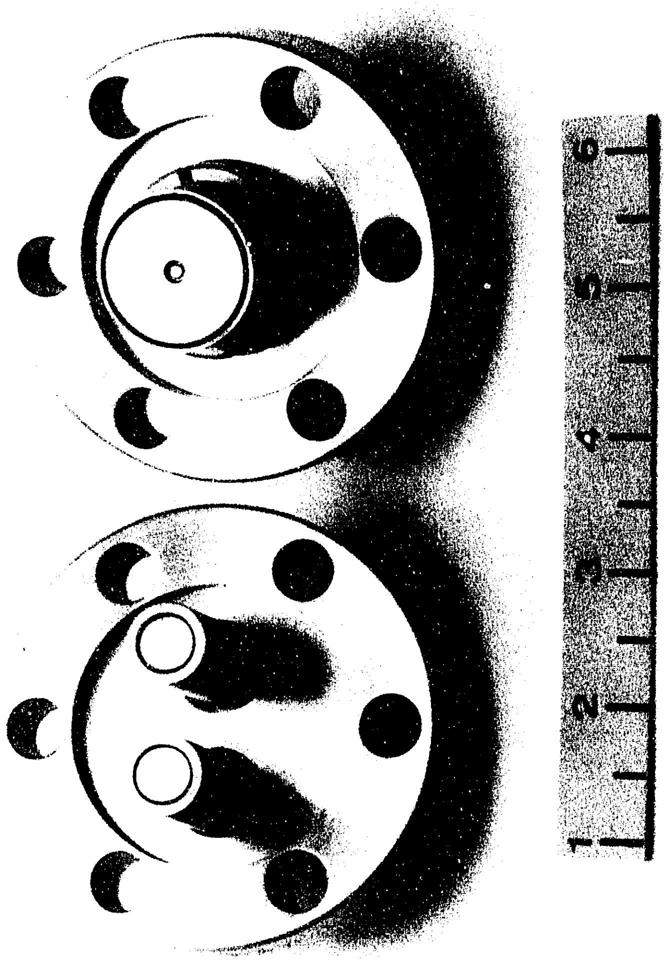
DC global absolute orbit correction at SPEAR, SSRL, using the algorithm of singular value decomposition (SVD). The r.m.s. orbit error relative to the vacuum chamber center is 780 µm and 215 µm before and after correction, respectively. (Collaboration with W. J. Corbett, SSRL, and M. J. Lee, SLAC).

Advanced Photon Source

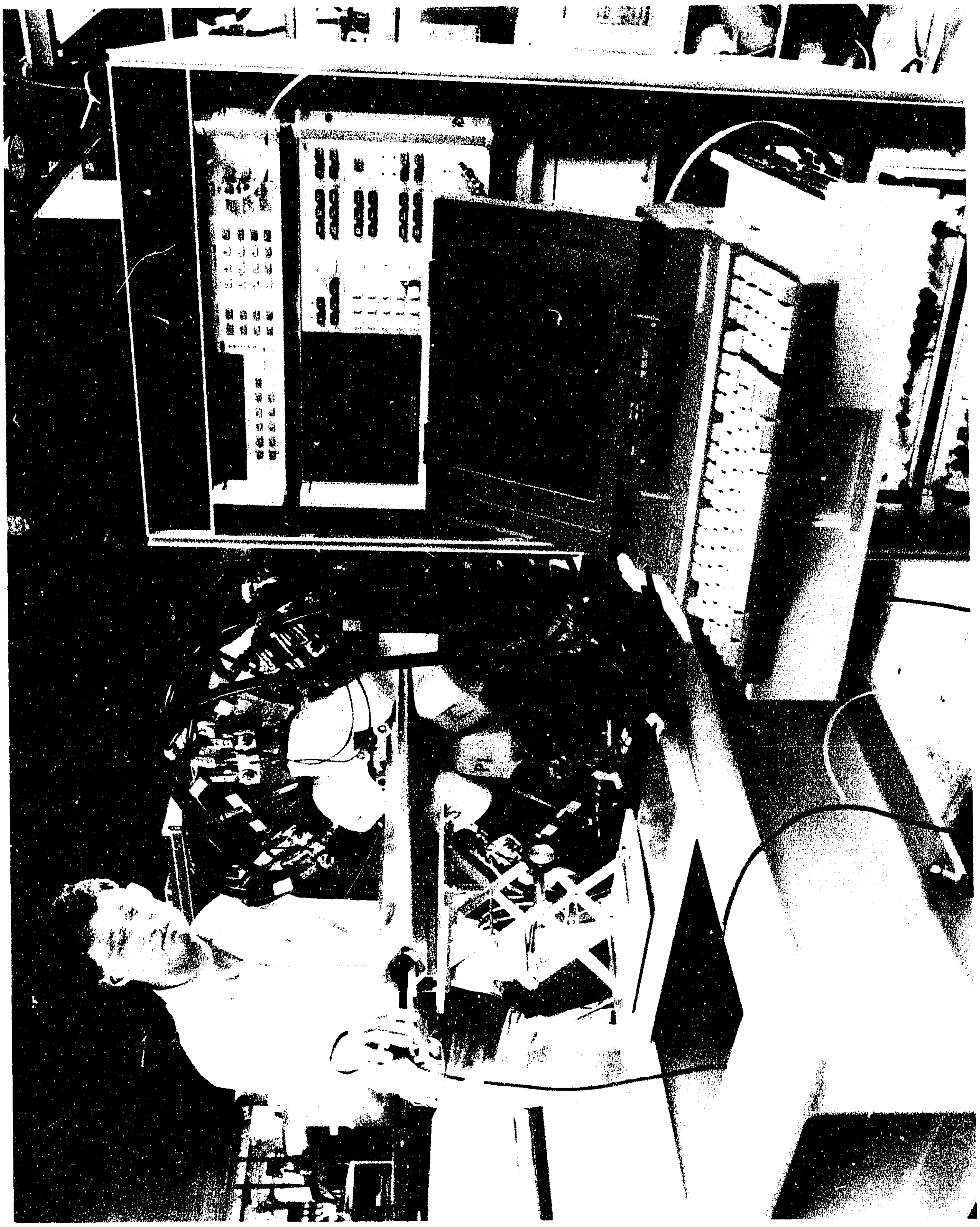


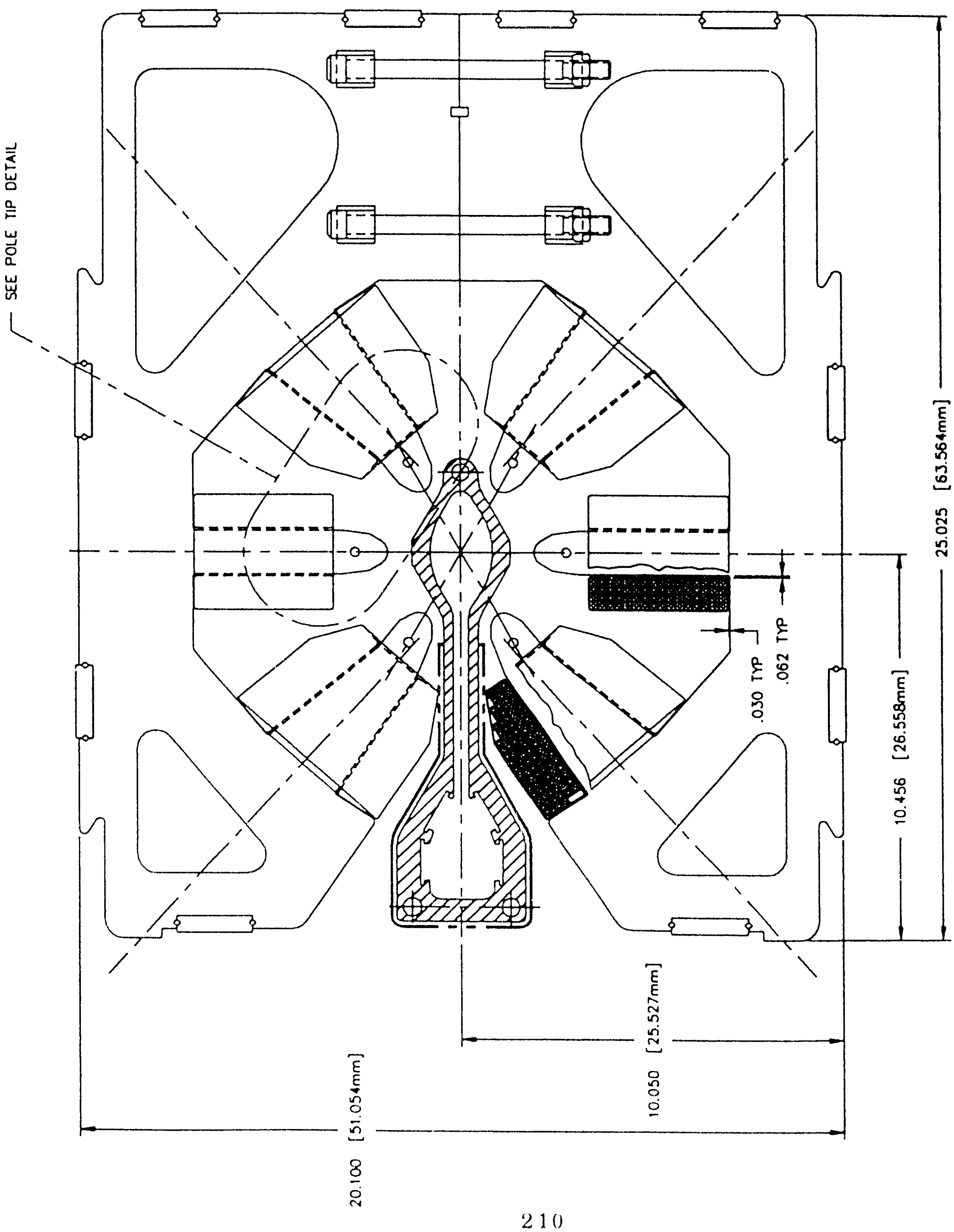
Schematic of Local Feedback System



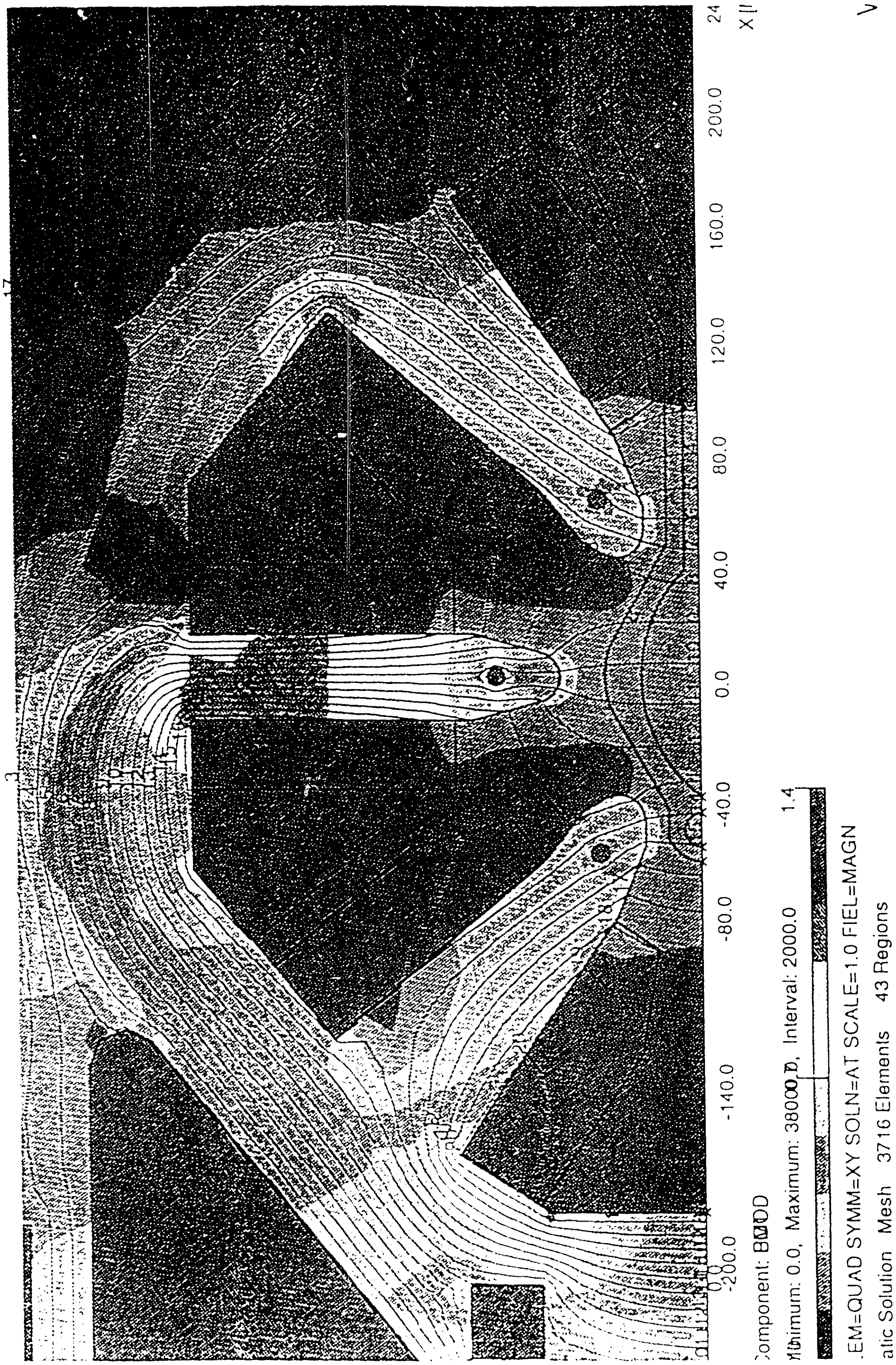

1
2
3
4
5
6

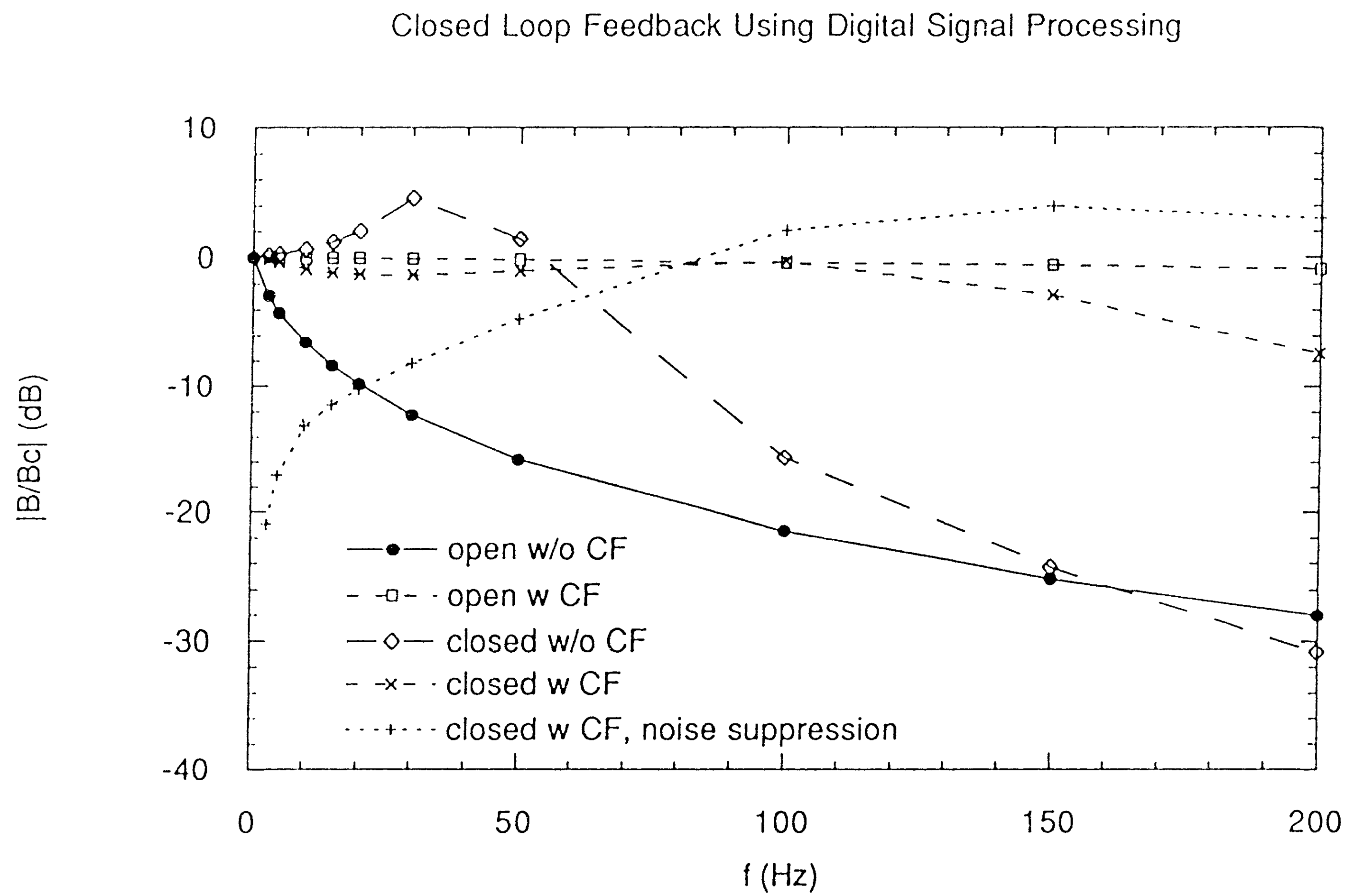

DIGITAL SAMPLING OSCILLOSCOPE



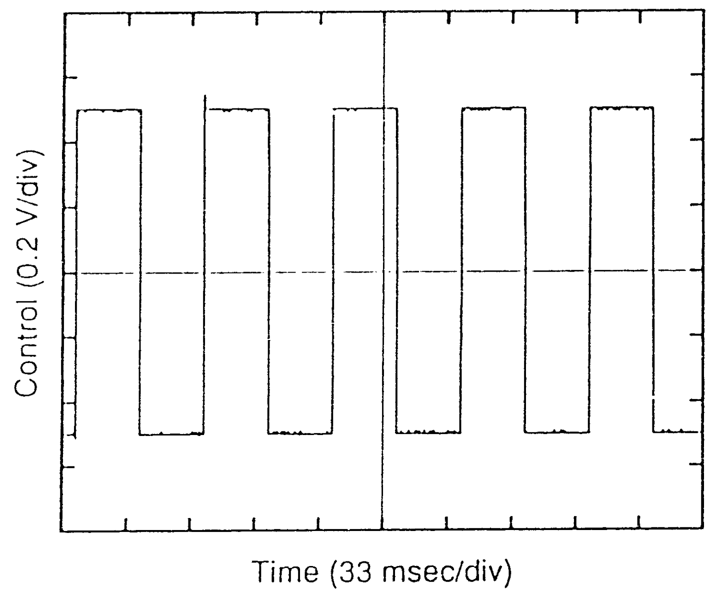


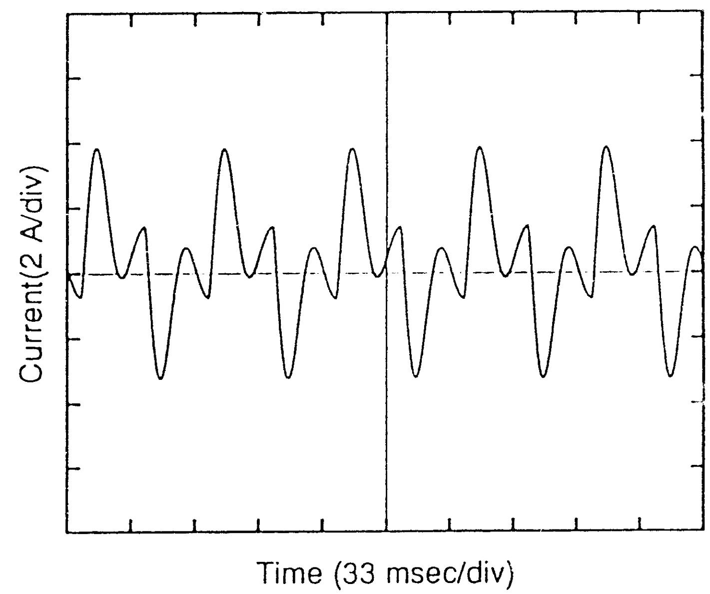
PROPOSED H/V CORRECTOR DESIGN

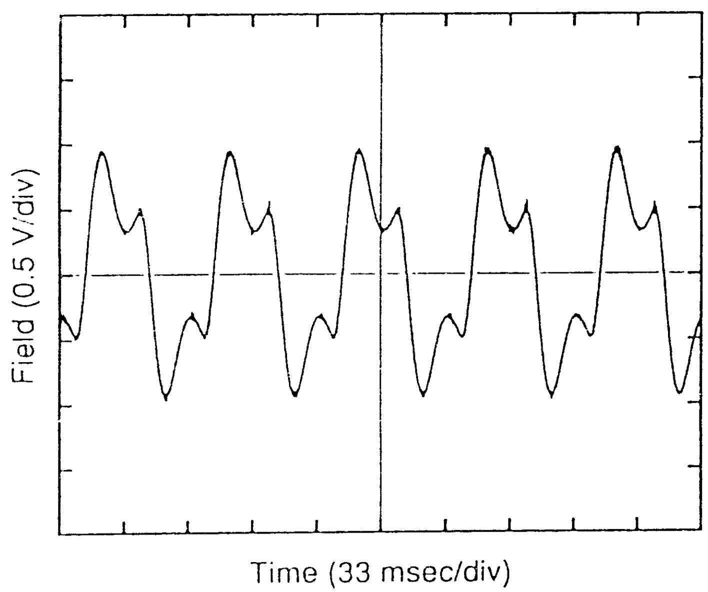

-200.0
-140.0
-80.0
-40.0
0.0
40.0
80.0
120.0
160.0
200.0
Interval: 2000.0
EM=QUAD SYMM=XY SOLN=AT SCALE=1.0 FIEL=MAGN
atic Solution Mesh 3716 Elements 43 Regions



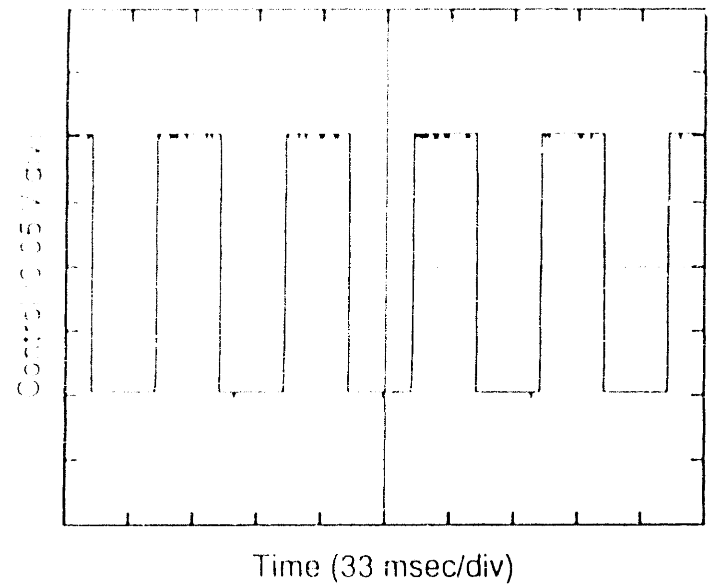
Transfer function of the closed loop feedback using PID control algorithm and digital signal processing for eddy current compensation. Power supply was in current-controlled mode and was bandlimited to 200 Hz. B_c is the control signal and B is the measured field in the storage ring VC.

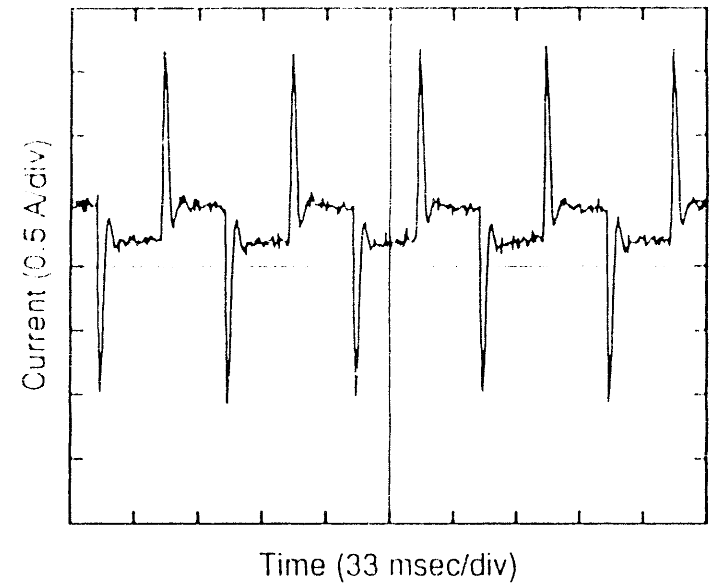


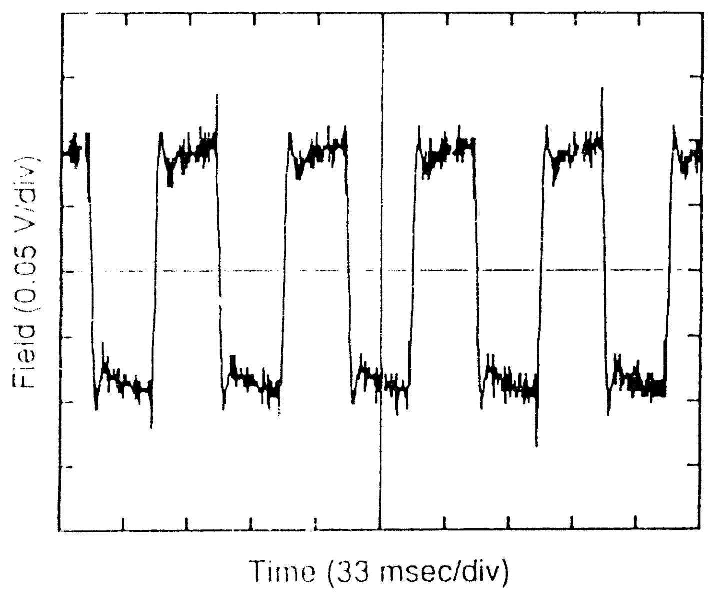




Closed loop feedback without eddy current compensation
Sampling frequency = 4 kHz
Square wave frequency = 15 Hz







Closed loop feedback with eddy current compensation
Sampling frequency = 4 kHz
Square wave frequency = 15 Hz

ADVANCED PHOTON SOURCE

PHOTON BEAM POSITION MONITOR DEVELOPMENT FOR APS FRONT ENDS

Tunch M. Kuzay

Beamline Engineering and Construction Group
Experimental Facilities Division

Fifth Users Meeting for the Advanced Photon Source
Argonne National Laboratory
Building 362

October 14-15, 1992

ADVANCED PHOTON SOURCE

Acknowledgements:

Experimental

Deming Shu

Juan Barraza

Tom Sanchez

Jeff Collins

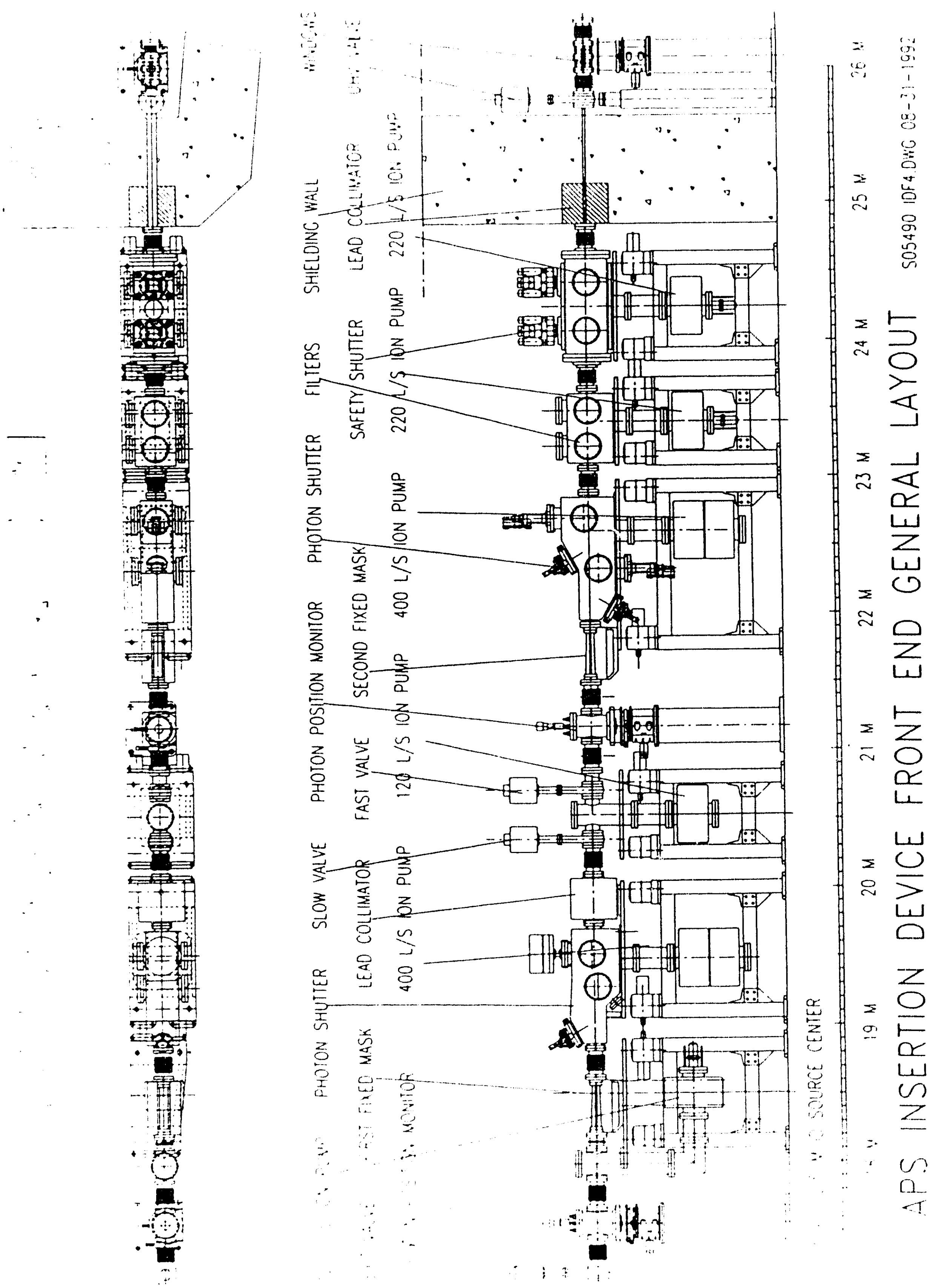
Brian Rodricks

CHESS and NSLS Beamline Staff

Analytical

Zhibi Wang

Tom Nian



SHIELDING WALL
LEAD COLLIMATOR
220 L/S ION PUMP
SAFETY SHUTTER
220 L/S ION PUMP
FILTERS
PHOTON SHUTTER
400 L/S ION PUMP
SECOND FIXED MASK
PHOTON POSITION MONITOR
120 L/S ION PUMP
FAST VALVE
SLOW VALVE
LEAD COLLIMATOR
400 L/S ION PUMP
PHOTON SHUTTER
FIRST FIXED MASK
SOURCE CENTER
19 M
20 M
21 M
22 M
23 M
24 M
25 M
26 M
APS INSERTION DEVICE FRONT END GENERAL LAYOUT
S05490 IDF4.DWG 08-31-1992

Photon Beam Position Monitors

Design Goal:

Sensing 10% of undulator beam opening angle and beam spatial size.

For β_x and β_y of 10 m,

$$\partial\sigma_y < 8 - 30\ \mu m$$

$$\partial\sigma_{y'} < 1 - 2\ \mu rad$$

The detection of such changes is achieved by using two photon BPMs with a spatial resolution of $\pm$ 1μ and separated by 3 - 4 m.

ADVANCED PHOTON SOURCE

Progression of the BPM Development

- Conventional Metal Blades

- Metal Coated Diamond Blades (DBPM)

  - APS Patent in Progress, 1991

- Transmitting Metal Coated Diamond Blades (TBPM)

  - APS patent in Progress, 1992

ADVANCED PHOTON SOURCE

APS PBPM Design Criteria

- Photo-Electron Emission Type
    - Proven Performance
    - High Sensitivity
- Coated CVD Diamond Blade
- Rolling Edge or Triangular-Bar Shape Blades to suit Horizontal Gap Adjustment for all IDs
- Use Blade Pairs to Design Out the Blade "Shadowing" Problem

ADVANCED PHOTON SOURCE

Novelties incorporated in the APS PBPM Designs

- Separate
  - Photo-emission
  - Base Material
- Base Electrical Isolation is not Critical
- Choice of Photo-Emission Coating Material Best Suited to the Need
- Thinner Blade Material

ADVANCED PHOTON SOURCE

Experimental BPM Programs:

DBPM (1991)

- X-13 Soft X-ray Undulator Tests at NSLS
- APS/Chess Undulator at Cornell

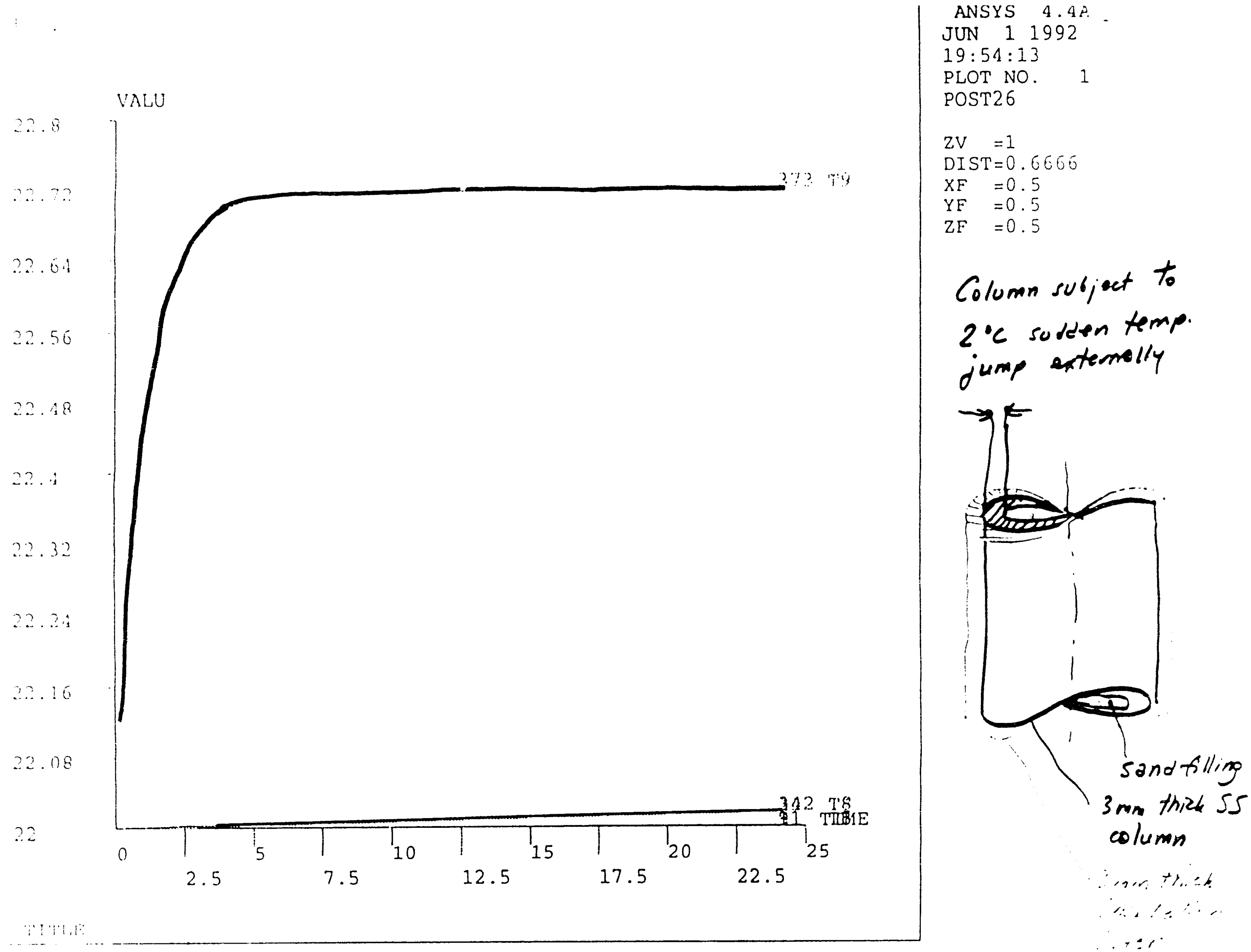
  4.3-7.9 keV energy band

TBPM (1992)

- X-25 Focused Wiggler at NSLS

Beam Position monitor Support Base Vertical Thermal Expansion for 1 ^{0}C Temperature Change

Case	Specification	Thermal Expansion
1	SS Cylinder	16.2 μm
2	SS Cylinder Filled with Water At Constant Temperature	0.82 μm
3	Case #2 with Ceramic Paper Insulation	0.33 μm
4	Ceramic Base Cylinder	0.50 μm

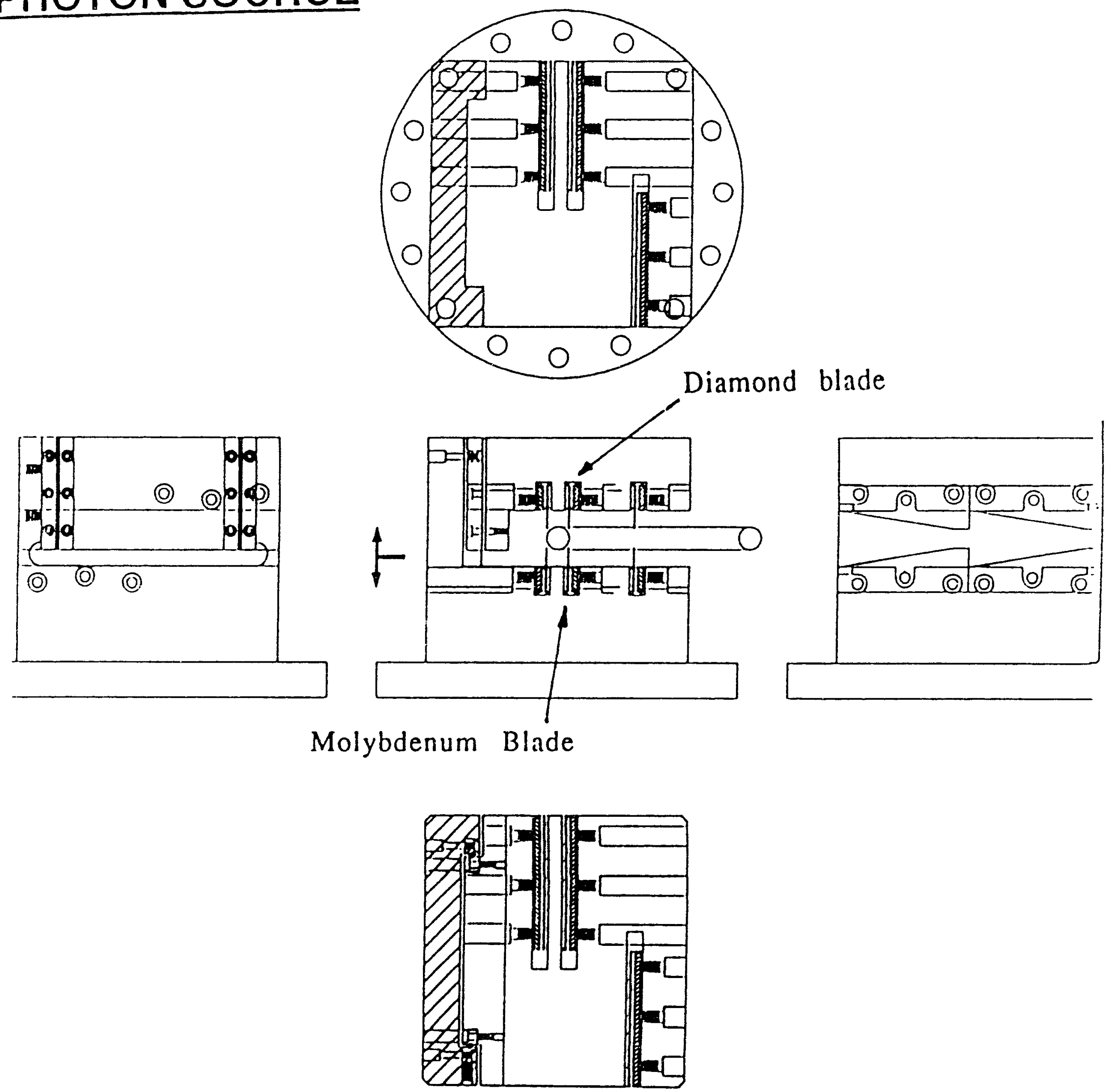


T along radius for SS cylinder filled with sand and covered with ceramic paper

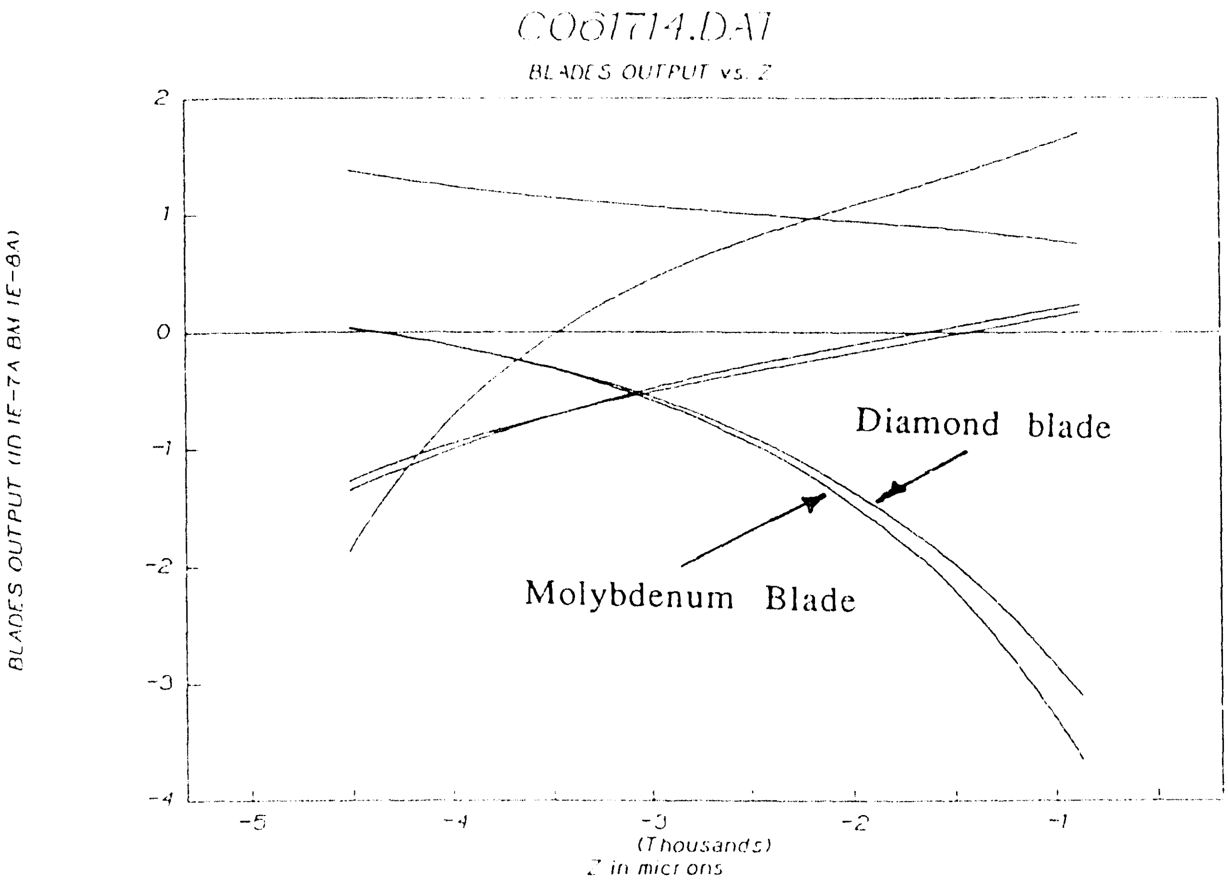
ADVANCED PHOTON SOURCE

Specification for Beam Position Monitor Support System

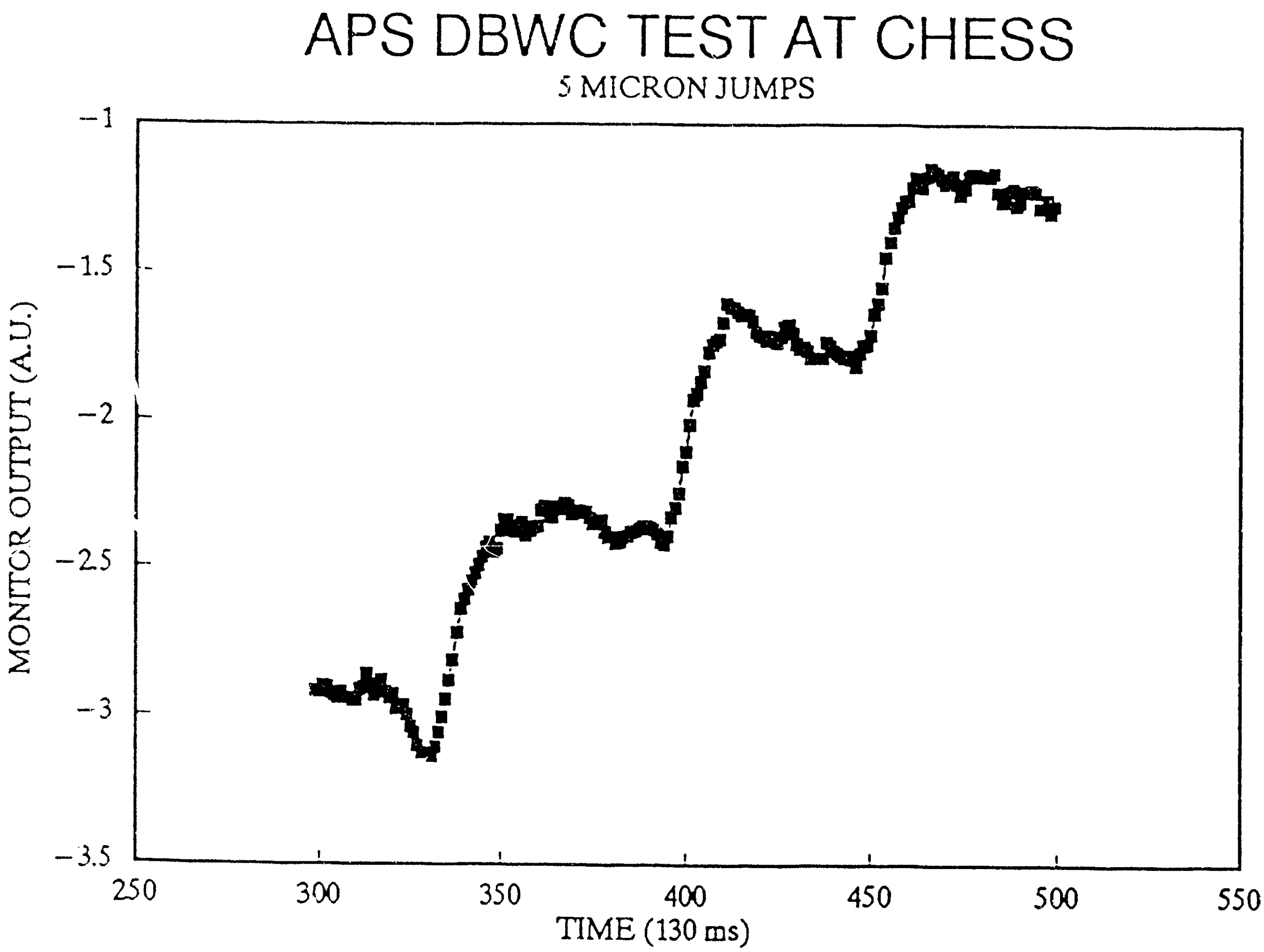
Maximum Load	100 lbs
Travel Range	± 5 mm
Resolution	0.5 -1 μm
Repeatability (horizontal)	± 5 μm
Repeatability (vertical)	± 2 μm
Maximum speed	0.5 mm/s
Staightness of Trajectory	10^{-5} rad/25 mm
Maximum deviation for 100 lbs offset	12.5 mm/10^{-5} rad



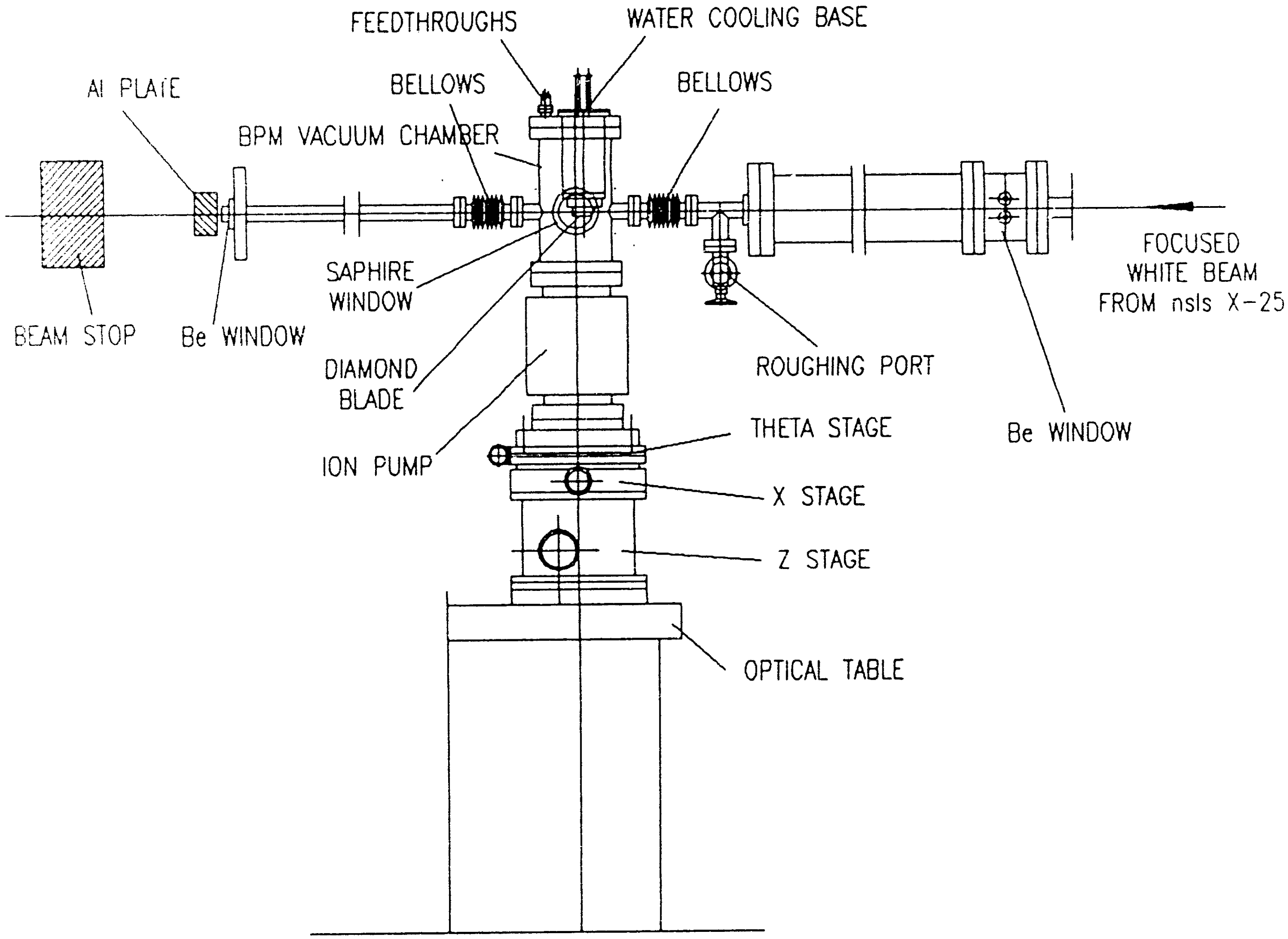
Assembly drawing of the Photon Beam Position Monitor
Tested at CHESS, Cornell University



Diamond and Molybdenum Blade photo-electron output tested at CHESS



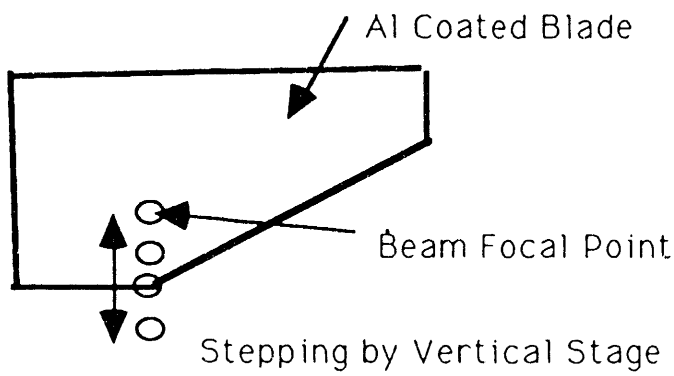
APS DBWC TEST AT CHESS
5 MICRON JUMPS
MONITOR OUTPUT (A.U.)
TIME (130 ms)
-1
-1.5
-2
-2.5
-3
-3.5
250
300
350
400
450
500
550

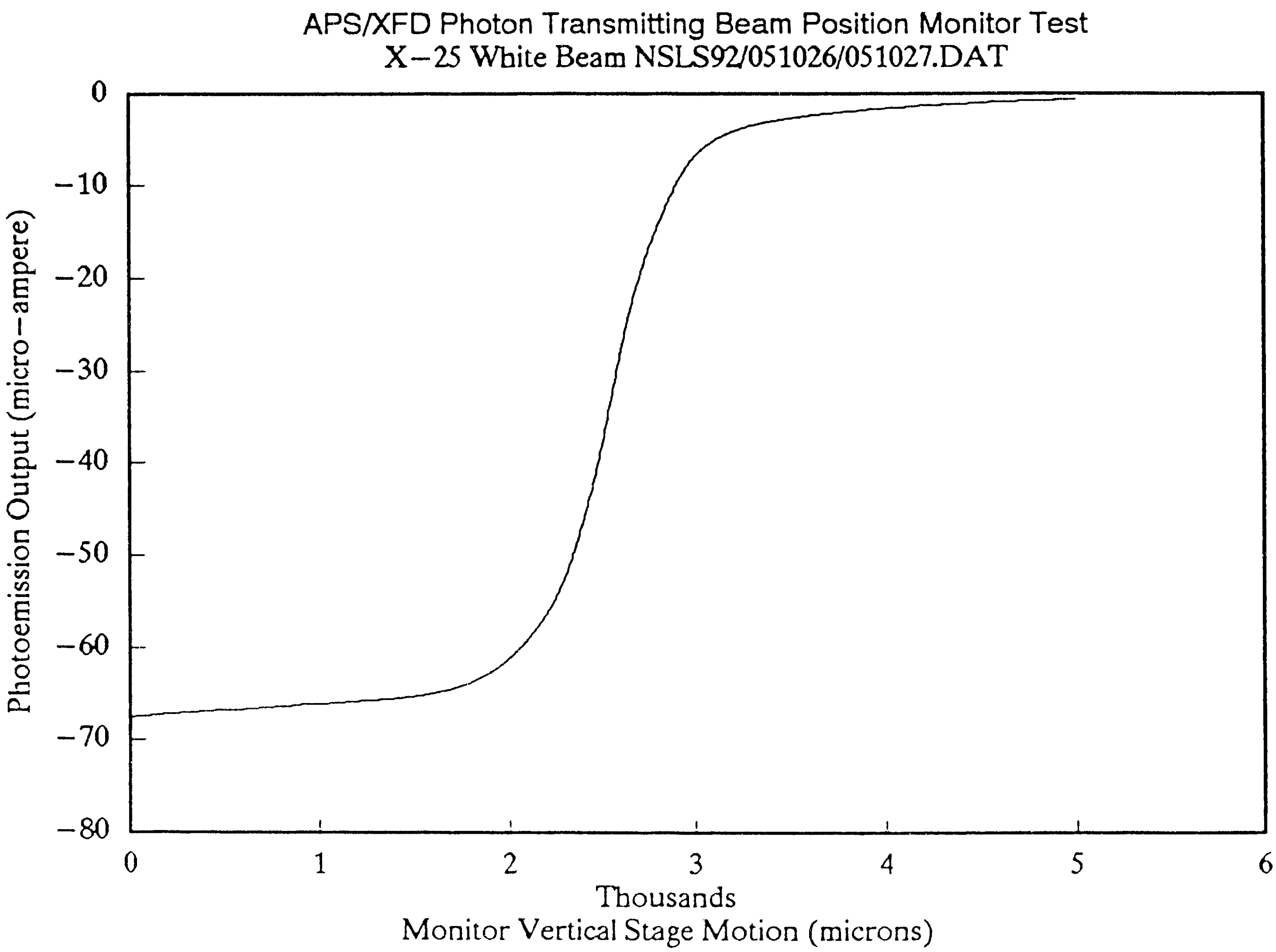


APS TBPM TEST SET-UP SCHEMATIC AT NSLS X-25

ADVANCED PHOTON SOURCE

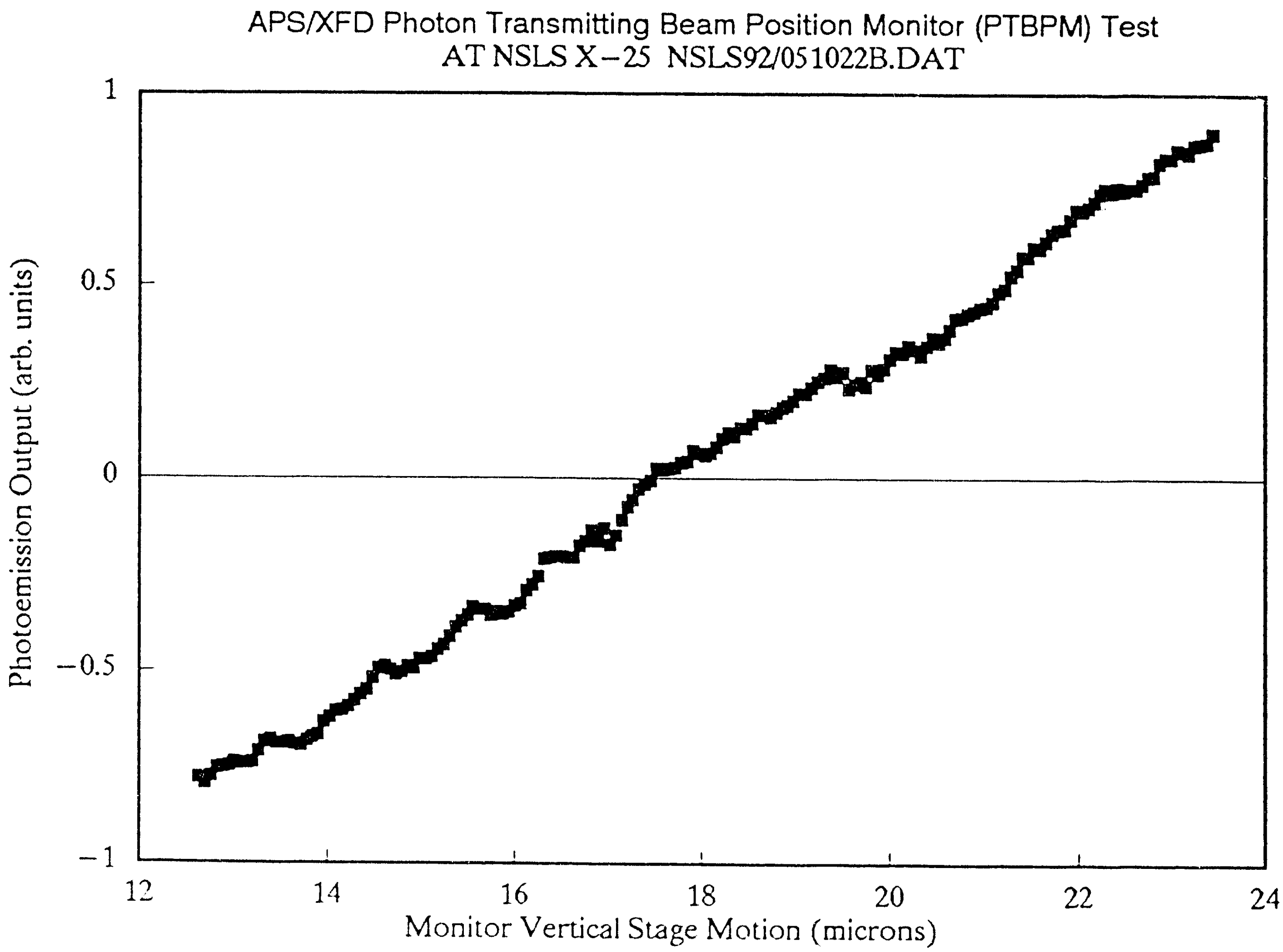
Vertical Stepping Tests at NSLS-X25



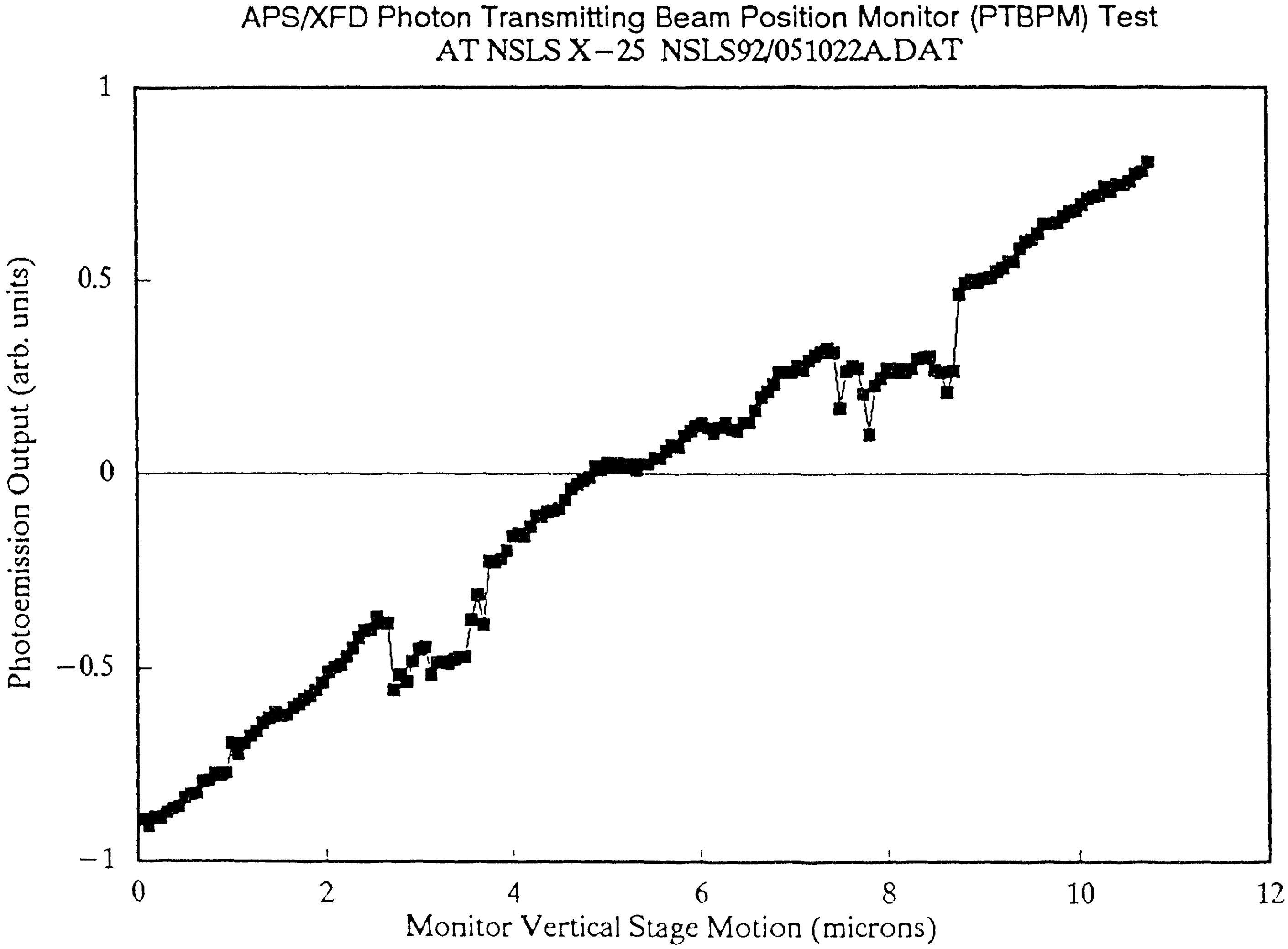


APS/XFD Photon Transmitting Beam Position Monitor Test
X−25 White Beam NSLS92/051026/051027.DAT
0
−10
−20
−30
−40
−50
−60
−70
−80
Photoemission Output (micro−ampere)
0
1
2
3
4
5
6
Thousands
Monitor Vertical Stage Motion (microns)

ADVANCED PHOTON SOURCE

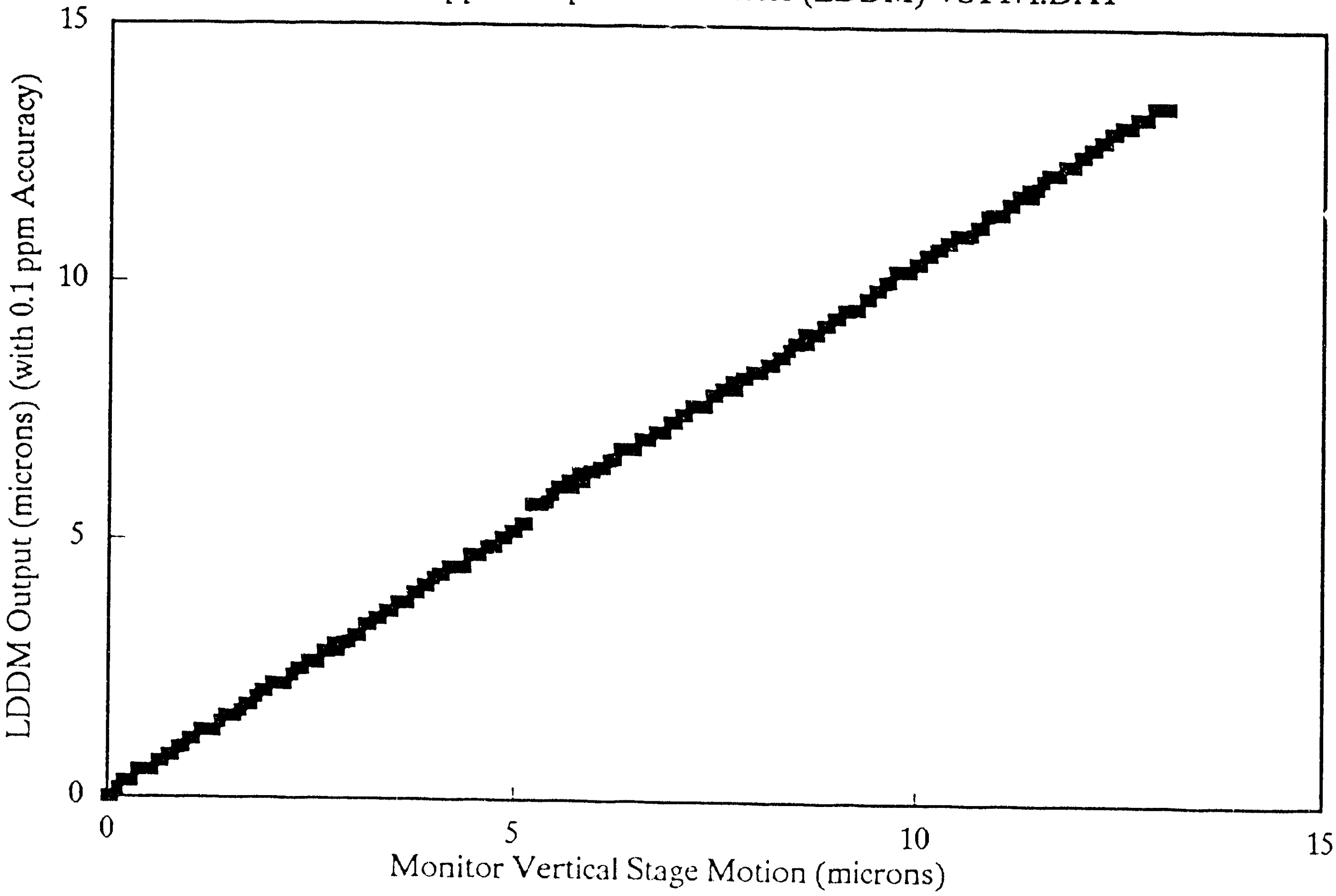


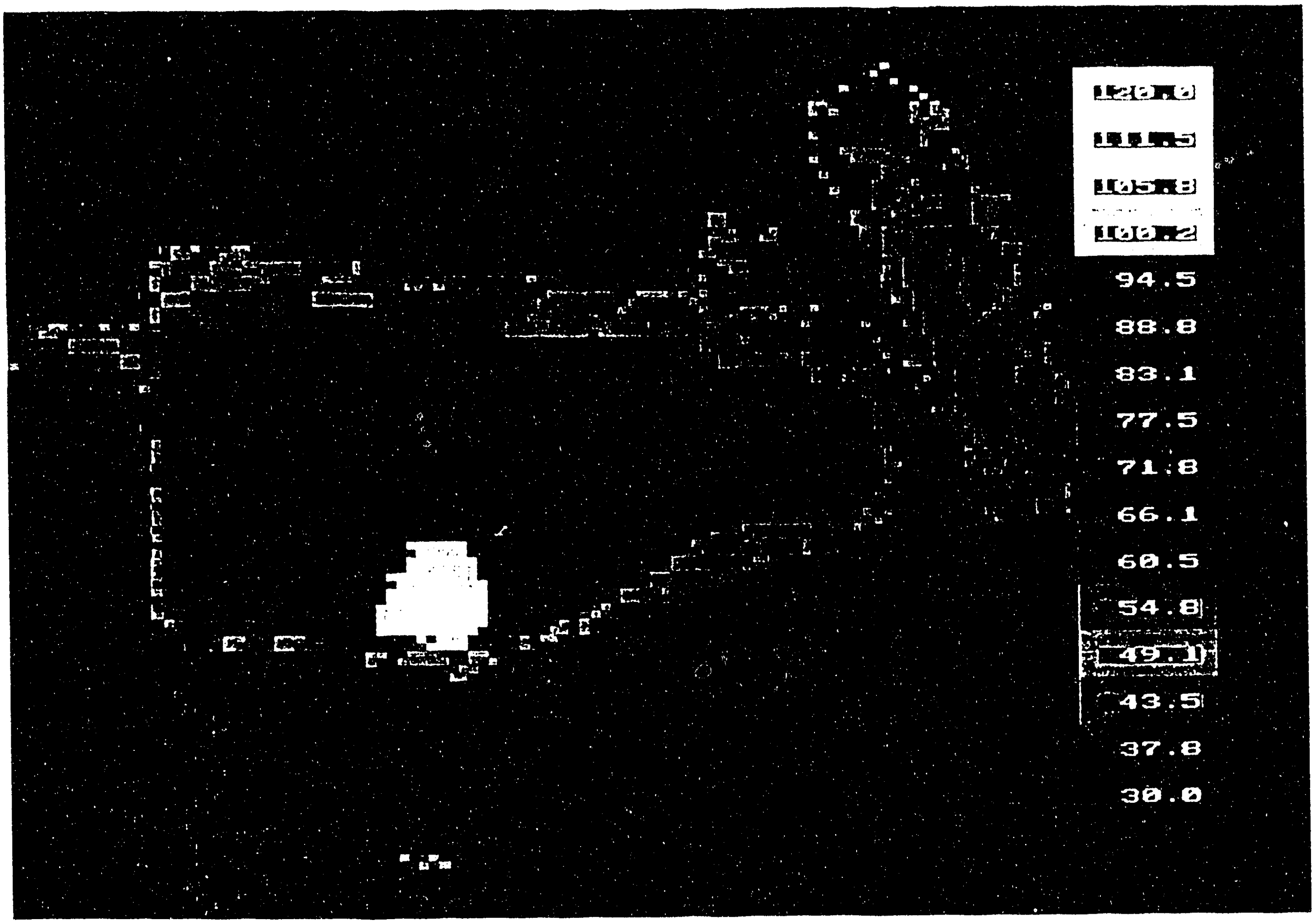
ADVANCED PHOTON SOURCE



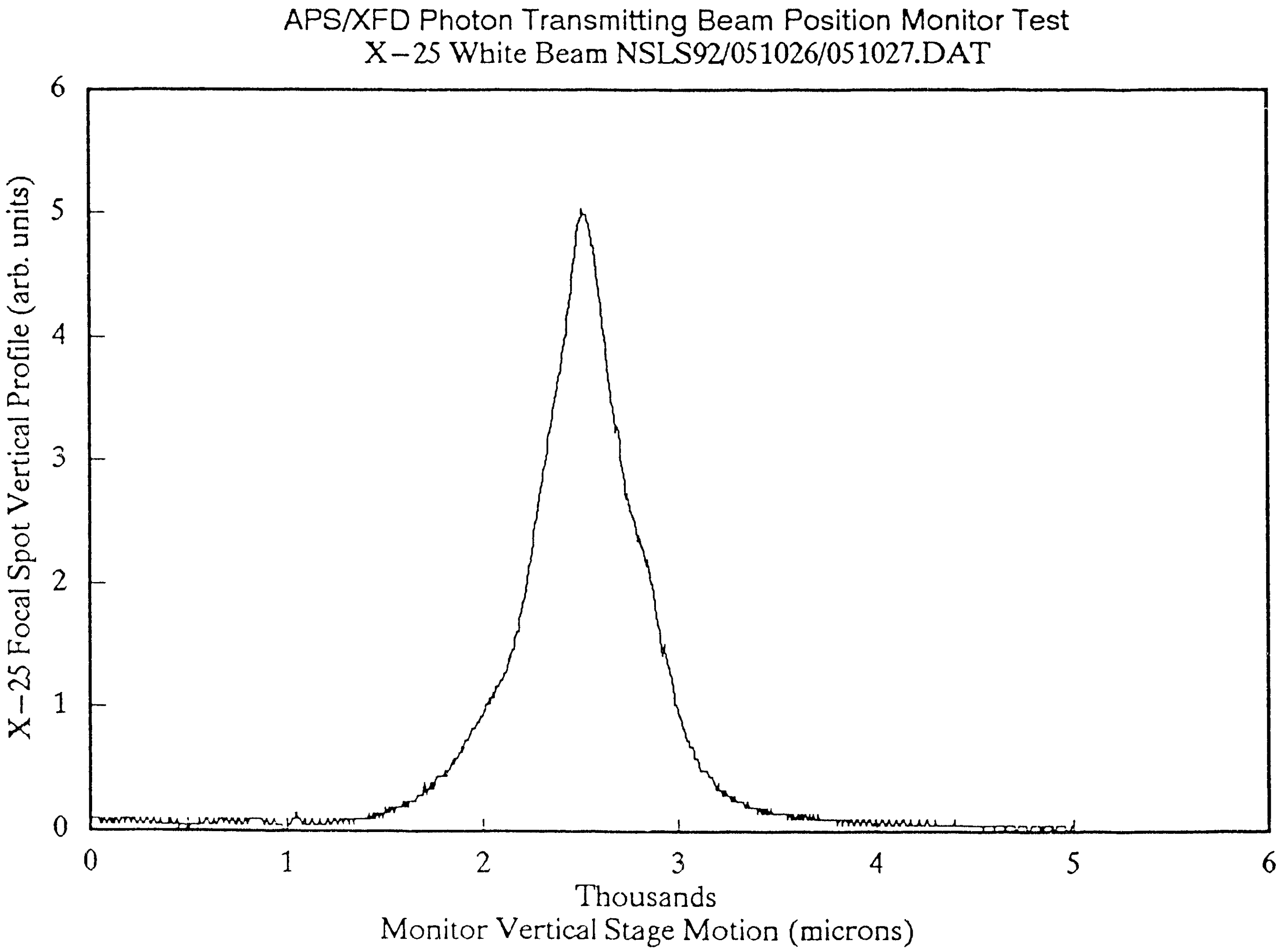
APS/XFD BPM Vertical Stage Test

Laser Doppler Displacement Meter (LDDM) VST171.DAT




120.0
111.5
105.8
100.2
94.5
88.8
83.1
77.5
71.8
66.1
60.5
54.8
49.1
43.5
37.8
30.0

ADVANCED PHOTON SOURCE



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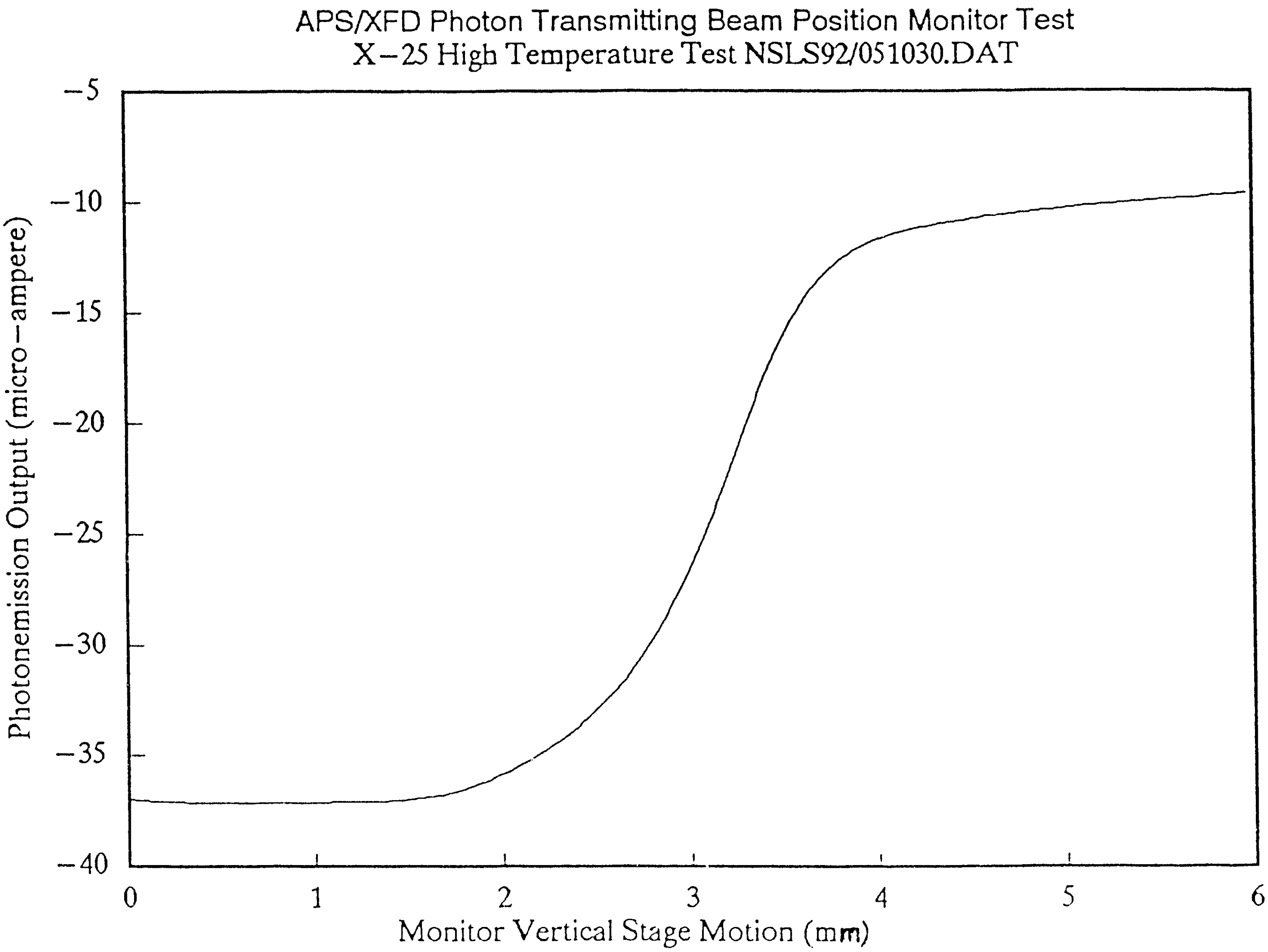
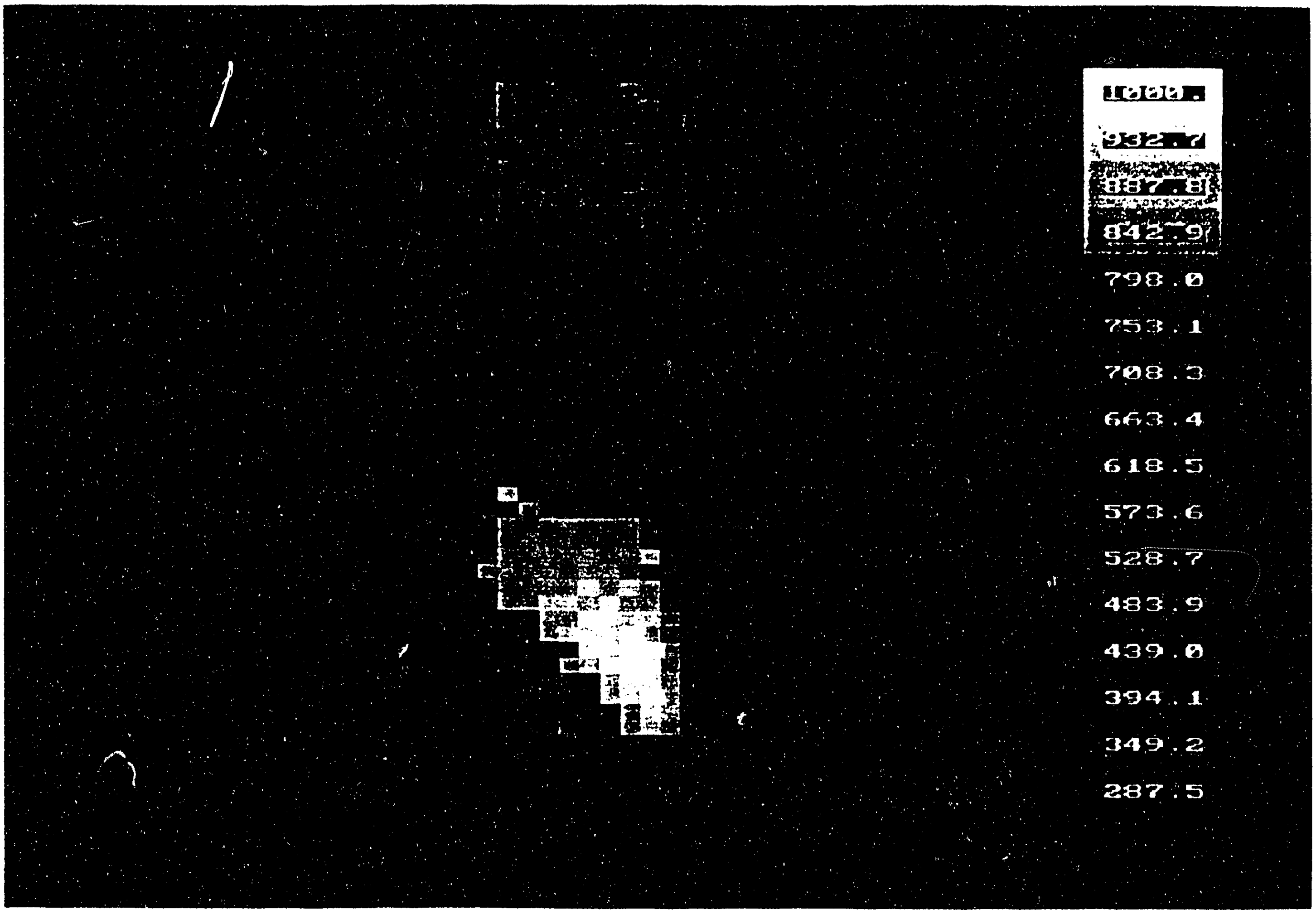
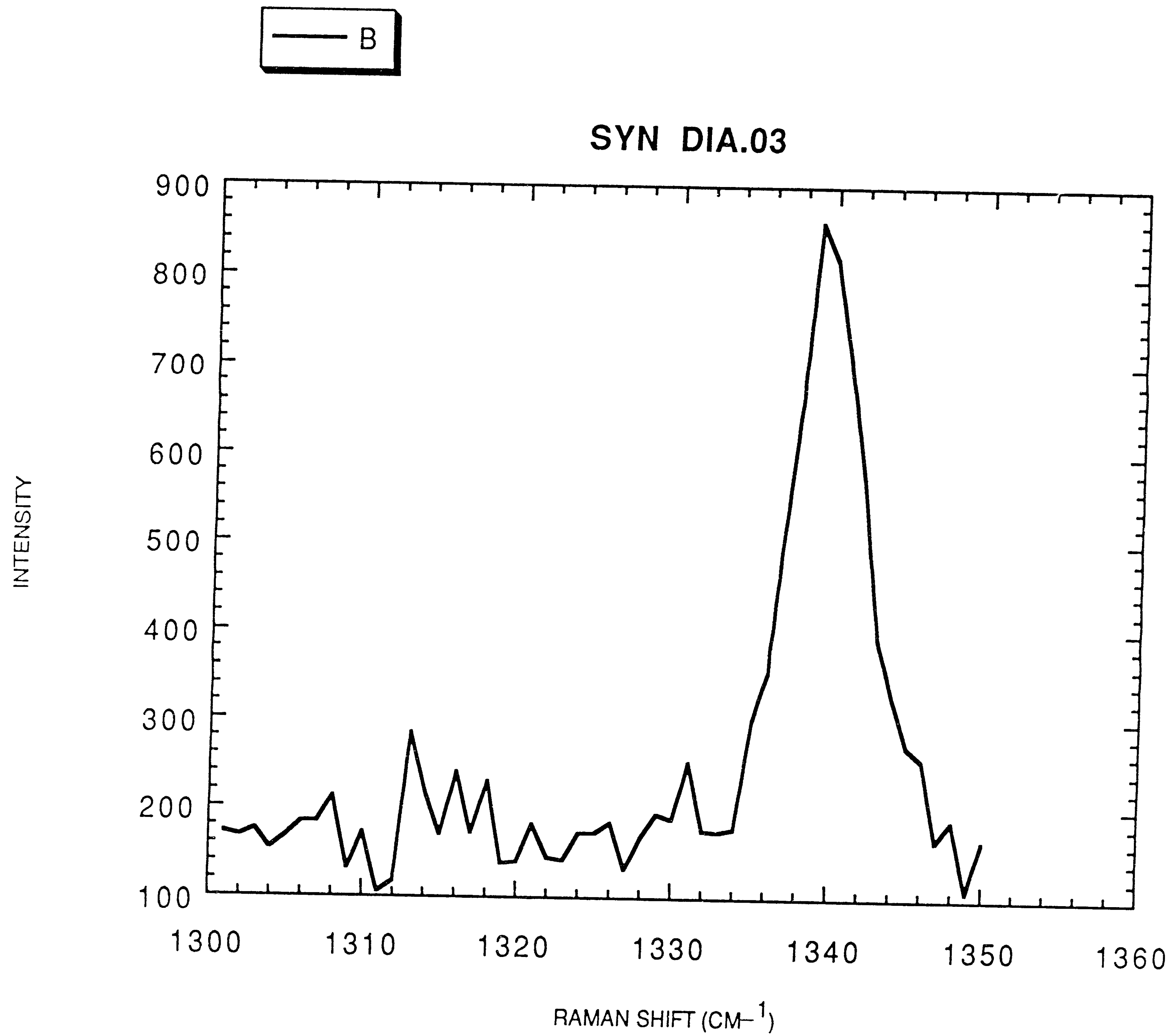
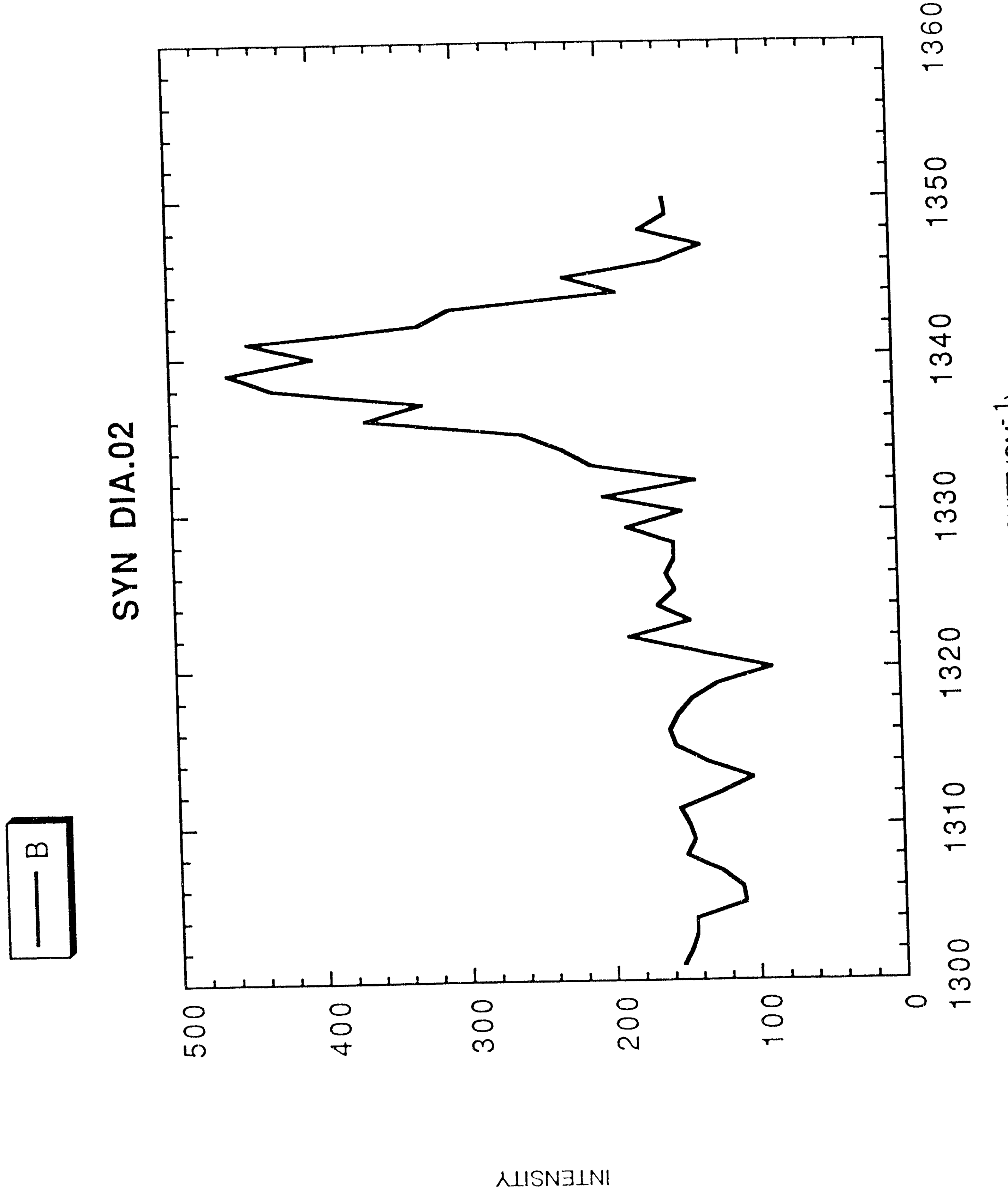
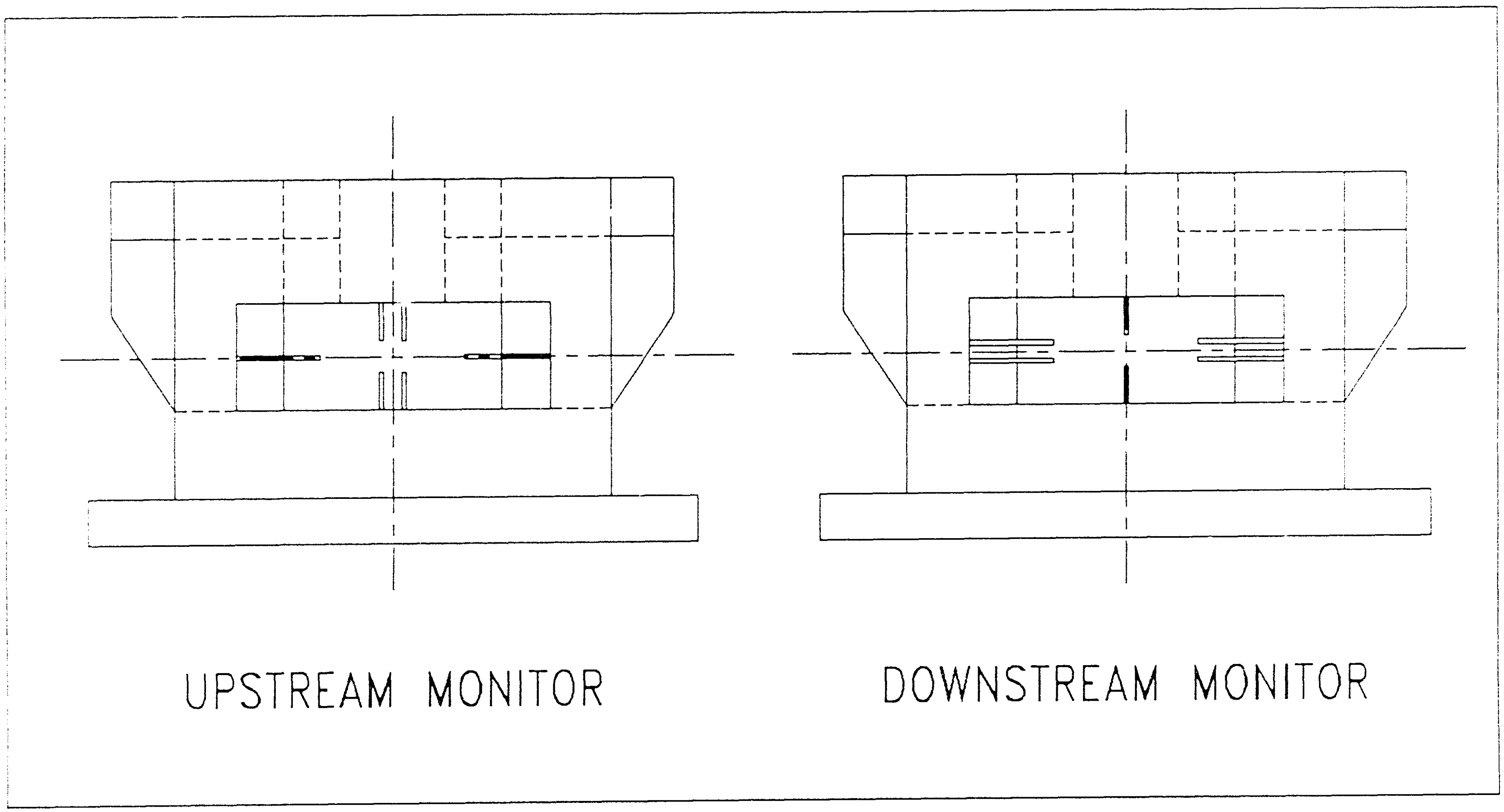


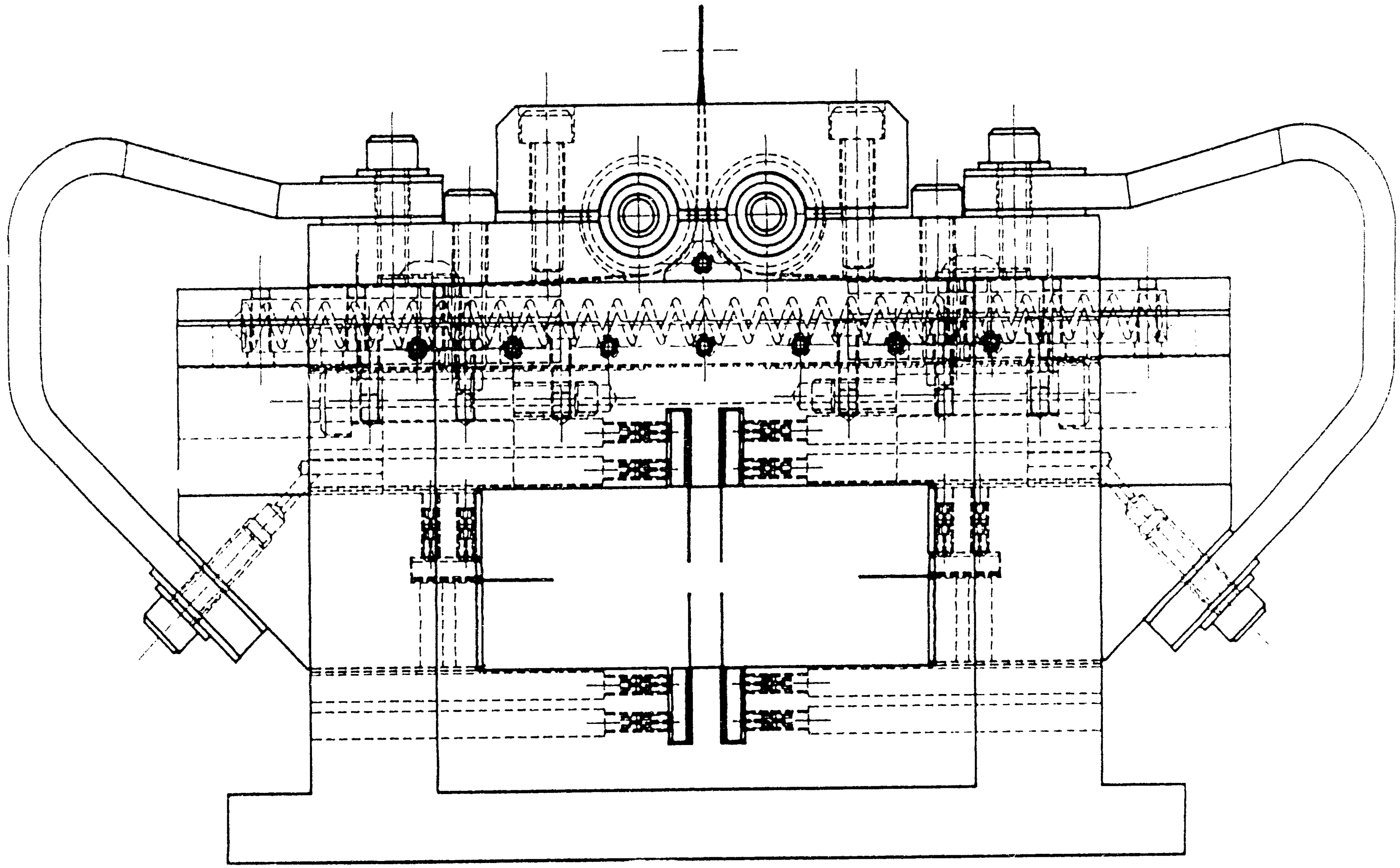

1000.
932.7
887.8
842.9
798.0
753.1
708.3
663.4
618.5
573.6
528.7
483.9
439.0
394.1
349.2
287.5


B
SYN DIA.03
INTENSITY
900
800
700
600
500
400
300
200
100
1300
1310
1320
1330
1340
1350
1360
RAMAN SHIFT (CM–1)


SYN DIA.02
B
INTENSITY
0
100
200
300
400
500
1300
1310
1320
1330
1340
1350
1360
RAMAN SHIFT (CM^-1)

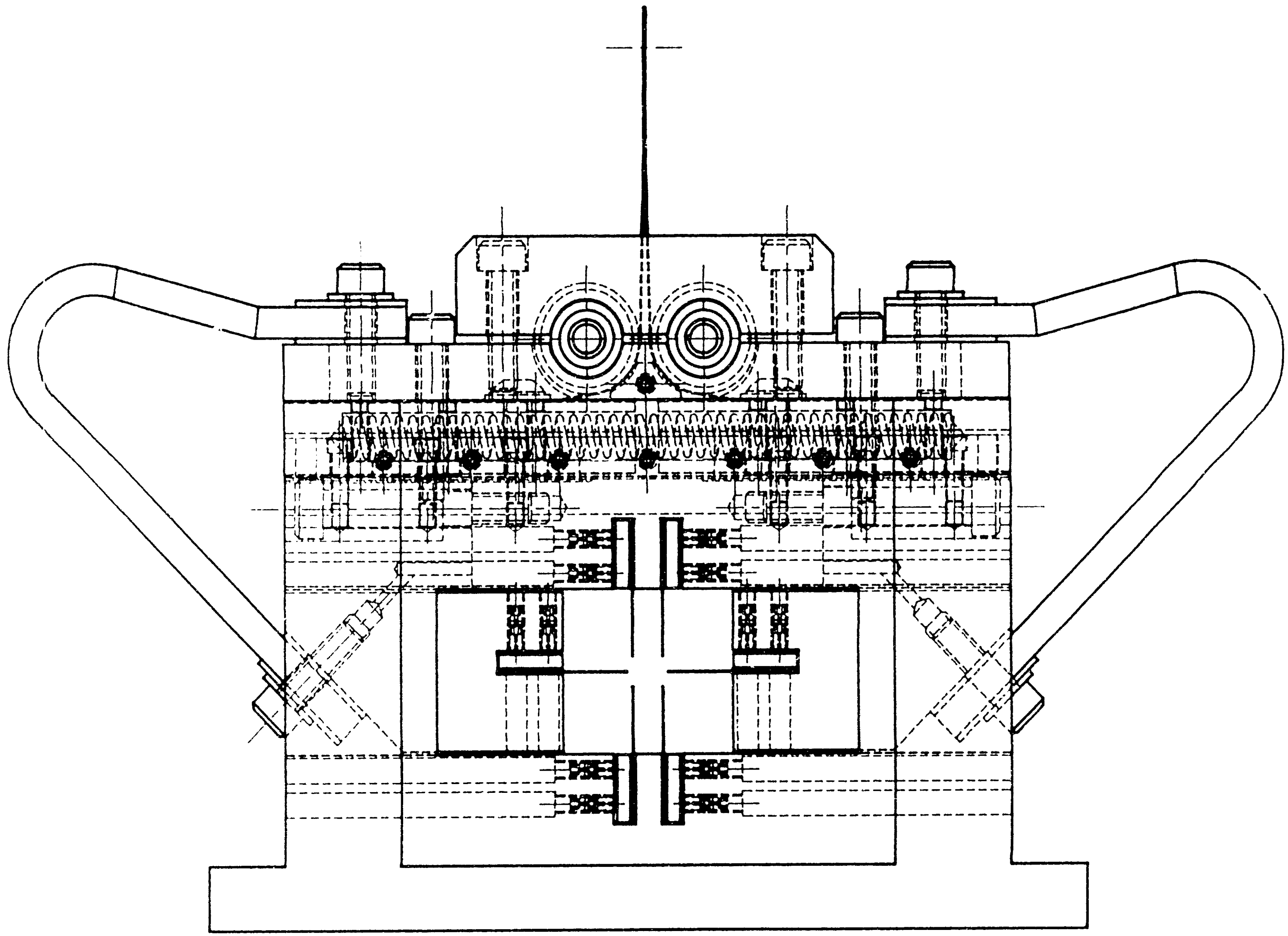

UPSTREAM MONITOR
DOWNSTREAM MONITOR

ADVANCED PHOTON SOURCE



IN OPEN POSITION

ADVANCED PHOTON SOURCE



IN CLOSED POSITION

Magnetic Field Measurements and Undulator Performance

J. Pflüger

APS/HASYLAB

Magnetic Field Measurements
and
Undulator Performance

Problem Description

In its final stage, the APS, a 7-GeV third generation synchrotron radiation source, will offer a total of 34 straight sections in which as many as 68 2.4-m-long insertion devices (IDs) can be installed. The basic principle of an ID using permanent magnets as well as soft iron pole pieces is shown in Fig. 1 (together with the coordinate system used).

Magnets are arranged so as to concentrate the magnetic flux via the soft iron pole pieces into the gap between the structure halves. Along the z axis, which is also the electron beam axis, the field varies sinusoidally. The magnetic field strength can easily be varied by changing the gap.

Figure 2 gives an impression how devices using this magnet technology may finally look. One of the x-ray wigglers installed in DORIS III at HASYLAB is shown. Figure 3 shows the brilliance of Undulator A planned for the APS. The figure shows the emitted spectrum of Undulator A at a small (11.5 mm) and a comparatively large (25 mm) gap. It is readily seen that the brilliance of the harmonics can be tuned in a given range by changing the gap.

The goal of magnetic measurement is therefore to:

a) assure compatibility with storage ring operation even if all 68 devices are used,
b) guarantee and check the quality of the emitted light.

Integral Field Properties

Here the interaction of an ID with the storage ring is of main interest. The ID can be considered a "black box" that changes the state of a transmitted electron beam as illustrated in Fig. 4. There might be a number of perturbing effects that can be detected through magnetic measurements. APS tolerances, which guarantee good operation of an ID, are shown in Fig. 5. They are taken from ref. [1].

Differential Field Properties

The quality of radiation as obtained from a specific device is the main interest here (see Fig. 6). The dominant equation, which determines the emission of light of an electron in a real magnetic field, is given by the radiation integral as found in ref. [2]. A detailed analysis of the field errors are given by Kincaid [3].

One quantity that is simple to derive is the optical phase. It is simply the difference of the exponential of the radiation integral between a real and an ideal trajectory.

Measurement Techniques

An overview of measurement techniques that will be available at the APS is given in Fig. 7. A magnetic bench suitable for Hall probe and moving coil measurements in both horizontal and vertical directions is already available and can be seen in Fig. 8.

Quick "on-the-fly" spectra as well as slow but accurate "point-by-point" data can be taken. The total travel along the electron beam axis is about 3.0 m. On such a bench, practically all magnetic quantities of interest can be determined. However, long coils allowing for quick and precise checks of field integral errors will also be made. They can be used "on site" in the storage ring. Rotating coils allow quick high precision measurements of magnetic multipoles. Data from both long and rotating coils can be thought of as complementary to the data that can be obtained with the magnetic bench.

Examples:

Figure 9 shows a field distribution along the electron beam axis of the wedged pole Undulator A prototype structure. It has 26 poles, a period length of 3.3 cm, and reaches a maximum field of 0.7 T at a gap of 11.5 mm. Figure 10 shows an example of the optical phase. Data from the SPring-8 prototype undulator, a device with almost identical magnetic parameters as Undulator A, are shown. The phase varies by only about ±2°, which is quite a good result. Figure 11 shows the calculated brightness of the third harmonic; a zero emittance beam and 7 GeV are assumed. One sees that the brightness of the third harmonic is reduced by about 30% although the magnetic performance of this device is quite high. Generally, higher harmonics are much more sensitive to field errors than the fundamental.

Field errors decrease the coherence of the radiation. Therefore, the intensity lost in the third harmonic is found at other energies. Figure 12 finally gives an impression how a real device like the SPring-8 prototype may perform at the APS with the appropriate emittence assumed. The change in peak shape is caused by the finite angular spread of the beam. Aside from a small shift in energy, which is an artifact of the calculation, there is about a 20% decrease in the intensity between ideal and real devices. Because the SPring-8 prototype can be considered an example of today's state-of-the-art magnet technology, the results give a good impression of what can be obtained with a real device at the APS.

Conclusion

The importance of the magnetic measuring techniques for both integral and differential measurements has been demonstrated. At the APS, all techniques required to verify the magnetic performance of IDs will be available.

The results with the SPring-8 prototype demonstrate how magnetic measurements can be used for optical characterization but also show the current state-of-the-art performance of IDs.

Literature

1. APS Design Report Undulator A Specification, Sept. 92
2. J.D. Jackson, *Classical Electrodynamics*, Chapter 12, John Wiley & Sons
3. B. Kincaid, *J. Opt. Soc. Am B* **2**, 1294 (1985)

Acknowledgements

Special thanks to members of the APS Insertion Device Group: E. Gluskin, J. Maines, L. Moog, J. O'Brien, and R. Savoy.

OVERVIEW

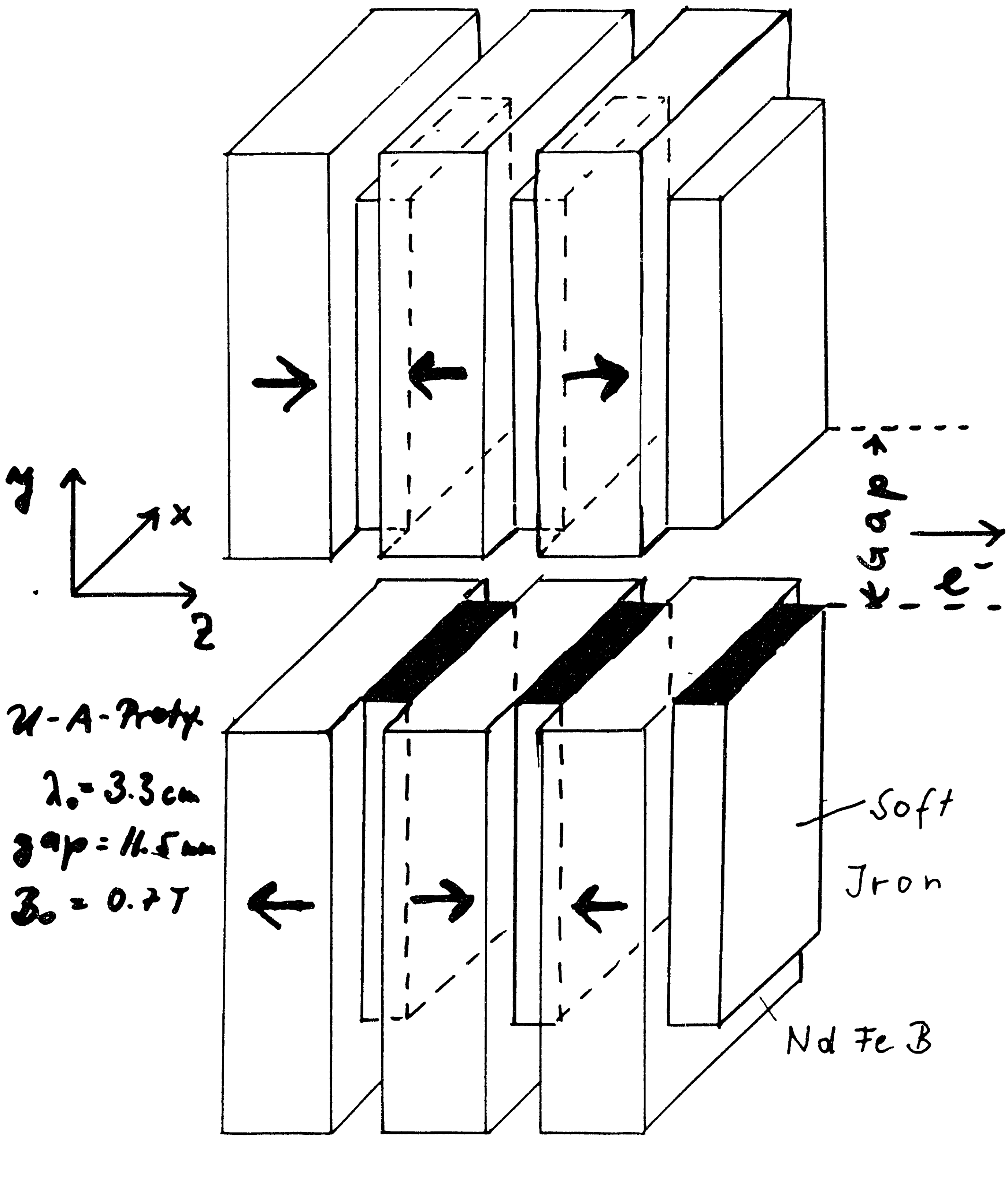
Problem Description

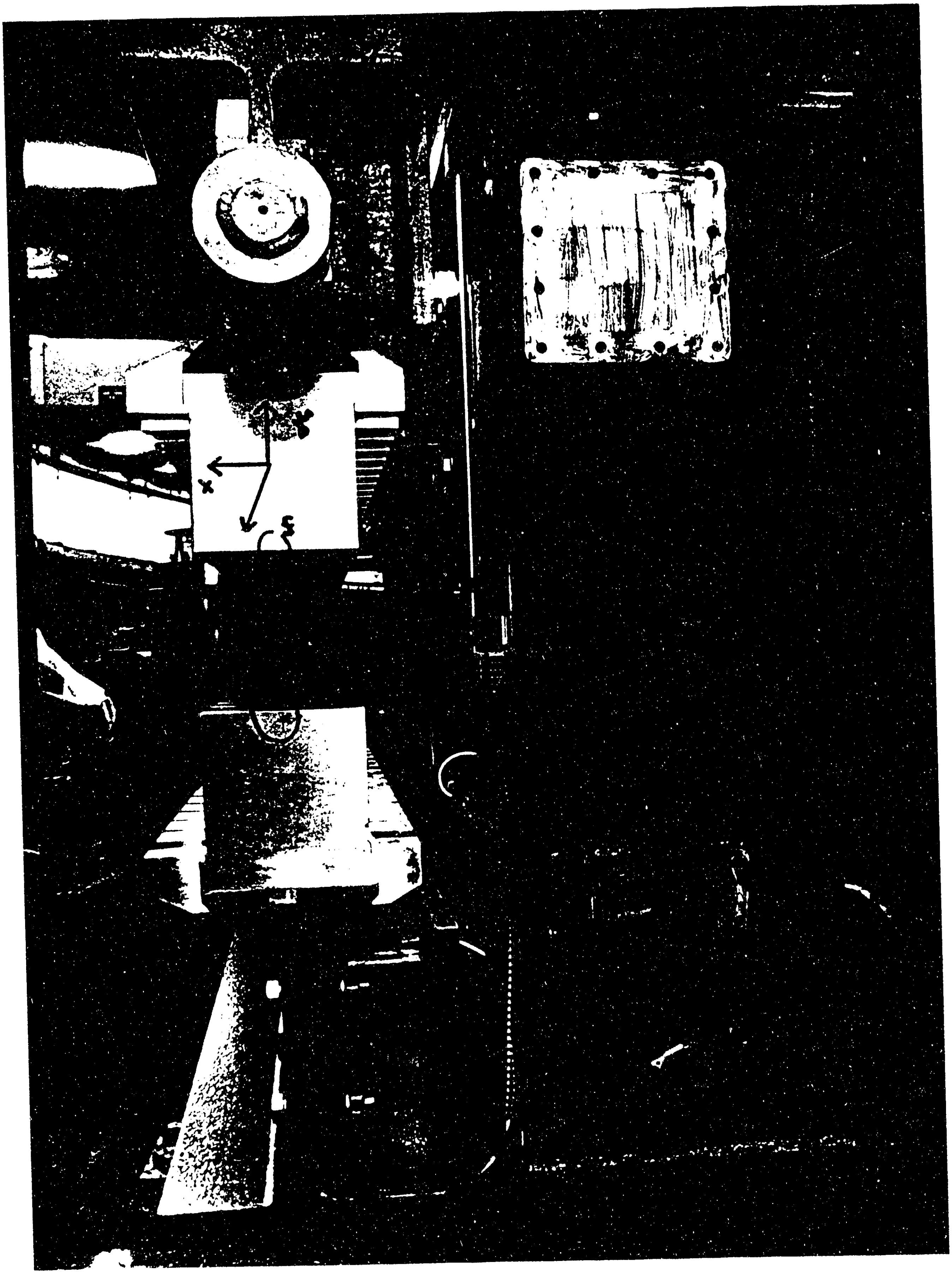
Integral Field Measurements
- Compatibility with Storage Ring Operation
- Magnetic Specs

Field Maps
- Individual Device Performance

Measurement Techniques (to be) Available at the APS

Some Examples
- APS U-A Prototype
- SPring 8 Prototype
- HASYLAB XUV 3


y
x
z
gap
e⁻
U-A-Proty
λ₀ = 3.3 cm
gap = 11.5 mm
B₀ = 0.7 T
Soft
Iron
Nd Fe B



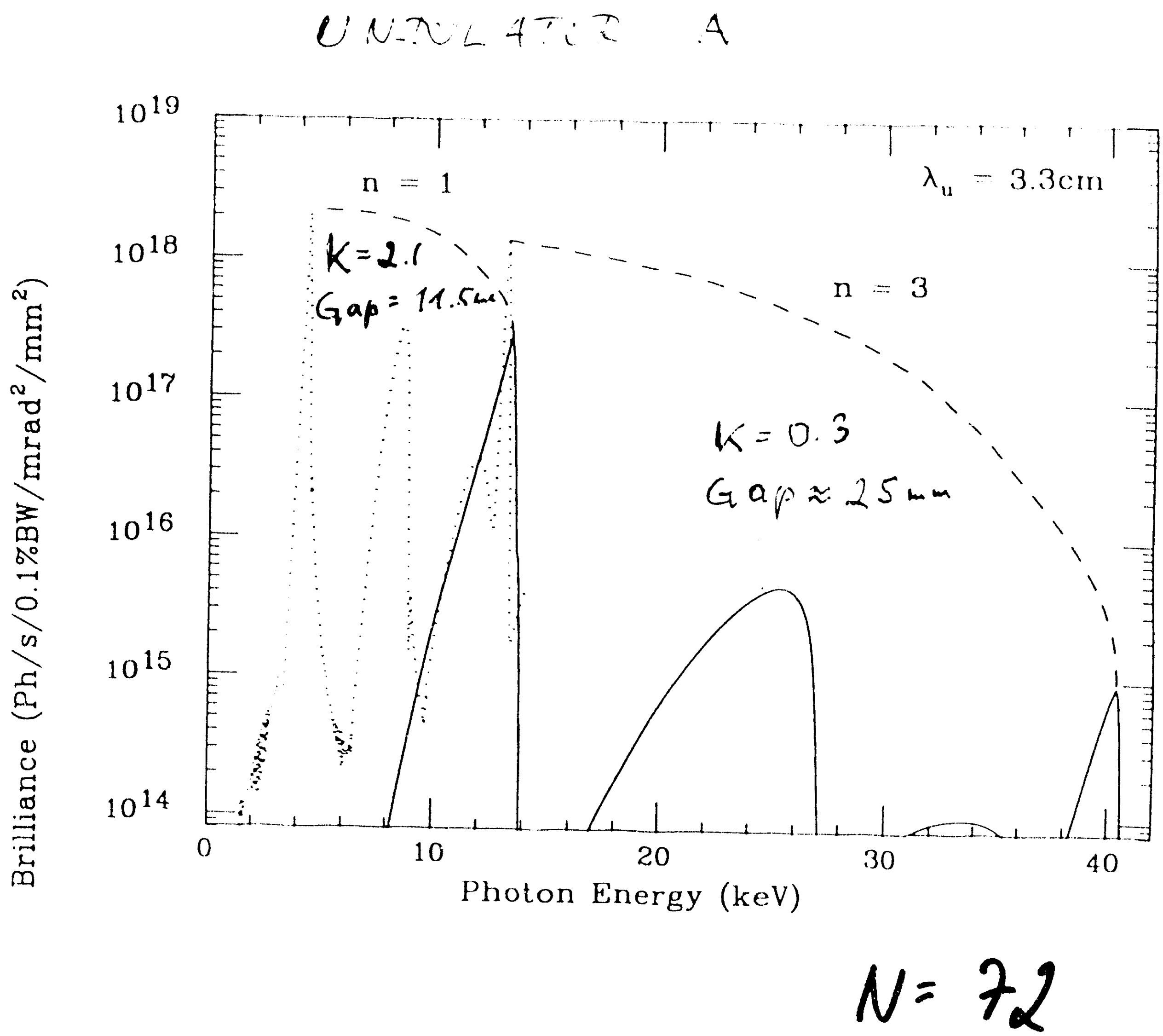
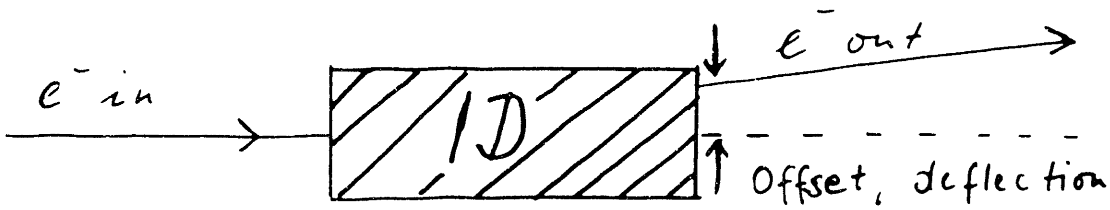


Fig. 3 On-axis brilliance of Undulator A. The spectral distribution of the first 3 harmonics are shown for the case of K = 0.3 (solid line) and K = 2.1 (dotted line). The overall envelope of the first and the third harmonic for the K-values in between are showed in dashed lines.

Integral Field Properties



Compatibility of up to 64 ID's with Storage Ring Operation

Required:

	Hor.	Ver
Offset [μm]	16	4.4
Deflec. Angle [μrad]	1.2	0.45

Determine:

Beam deflection	Hor. / Ver	1. Fieldint.
Beam displacement	Hor / Ver	2. Fieldint.
Tune shifts		Quadrupoles
Coupling of Hor / Ver Motion		Skew Quads
Limiting Dynamic Aperture		Sextupoles Octupoles

APS Magnetic Specs

Glenn Decker

1. Hor. Fieldint.	100 Gauss·cm
1. Ver. Fieldint.	100 Gauss·cm
2. Hor. Fieldint.	100.000 Gauss·cm^2
2. Ver. Fieldint	100.000 Gausscm^2
Integrated Quad.	50 Gauss
Int. Skew Quad.	50 Gauss
Integrated Sext.	200 Gauss/cm
Integrated Octup.	300 Gauss/cm^2
Int. Skew octup.	50 Gauss/cm^2

"Differential" Field Properties

Quality of Radiation of an individual Device

Dominant equ.

$$B_{ri}(\omega) = \text{const} \int_{-\infty}^{\infty} \vec{n} \times (\vec{n} \times \vec{\beta})\, e^{-i\omega(t - \vec{n}\vec{r}(t)/c)}\, dt$$

Jackson

Kincaid (1985) J. Opt. Soc. Am B 2 (1294)

Detailed Field distribution required

Calculation of optical Spectra

Optical Phase Definition

$$\Delta \varphi(z) = \frac{2\pi}{\lambda_R} \vec{n} \left(\vec{r}_{real} - \vec{r}_{ideal} \right)$$

Measurement Techniques
(to be)
available at the APS

Magnetic Bench for hor./Vert Hallprobe
and/or moving Coil Measurement

Field distributions, Field errors

Hor/Vert. Fieldintegrals, Multipoles complete

Long Coils Dipole Errors, "Steering" in Preparation

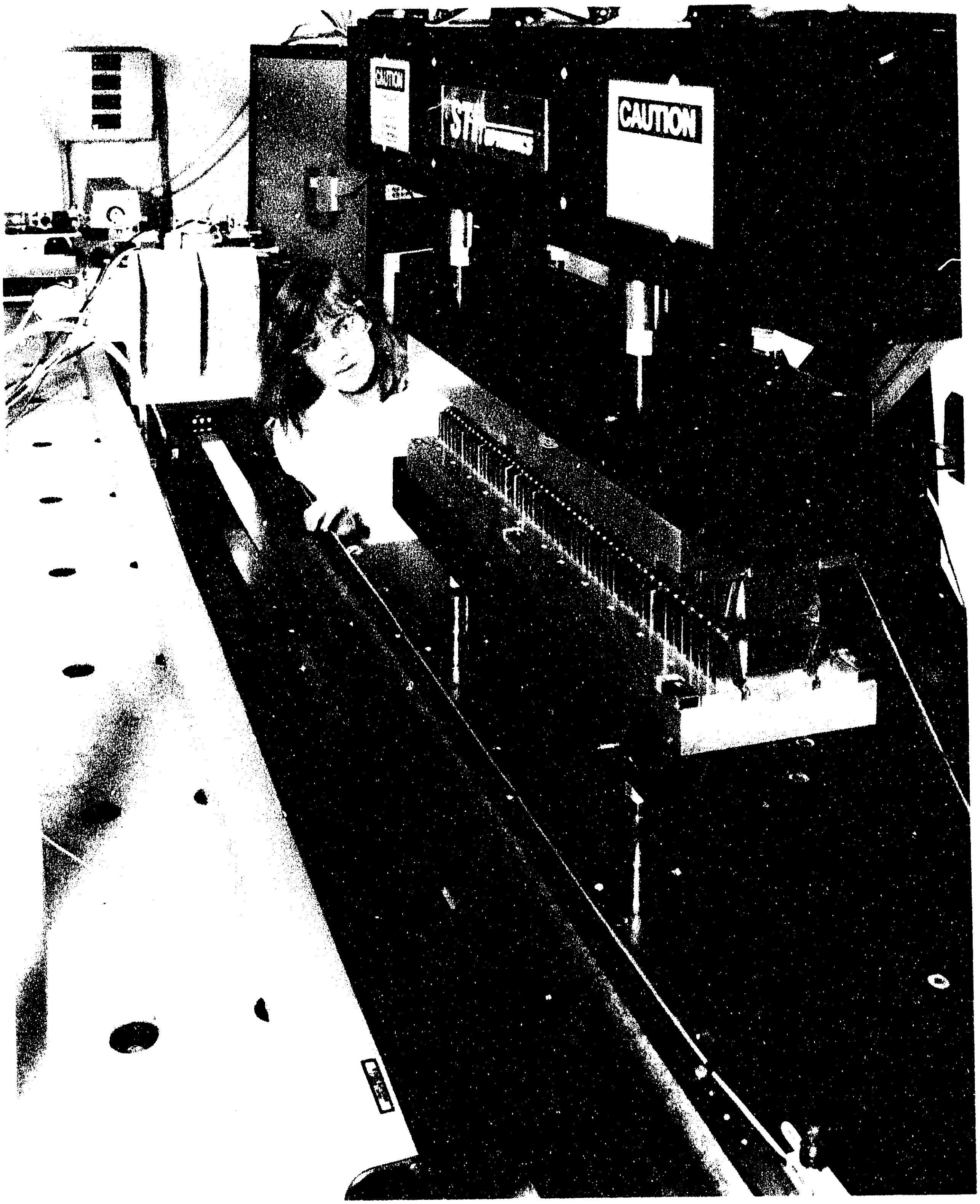
Rotating Long Coils Prototype

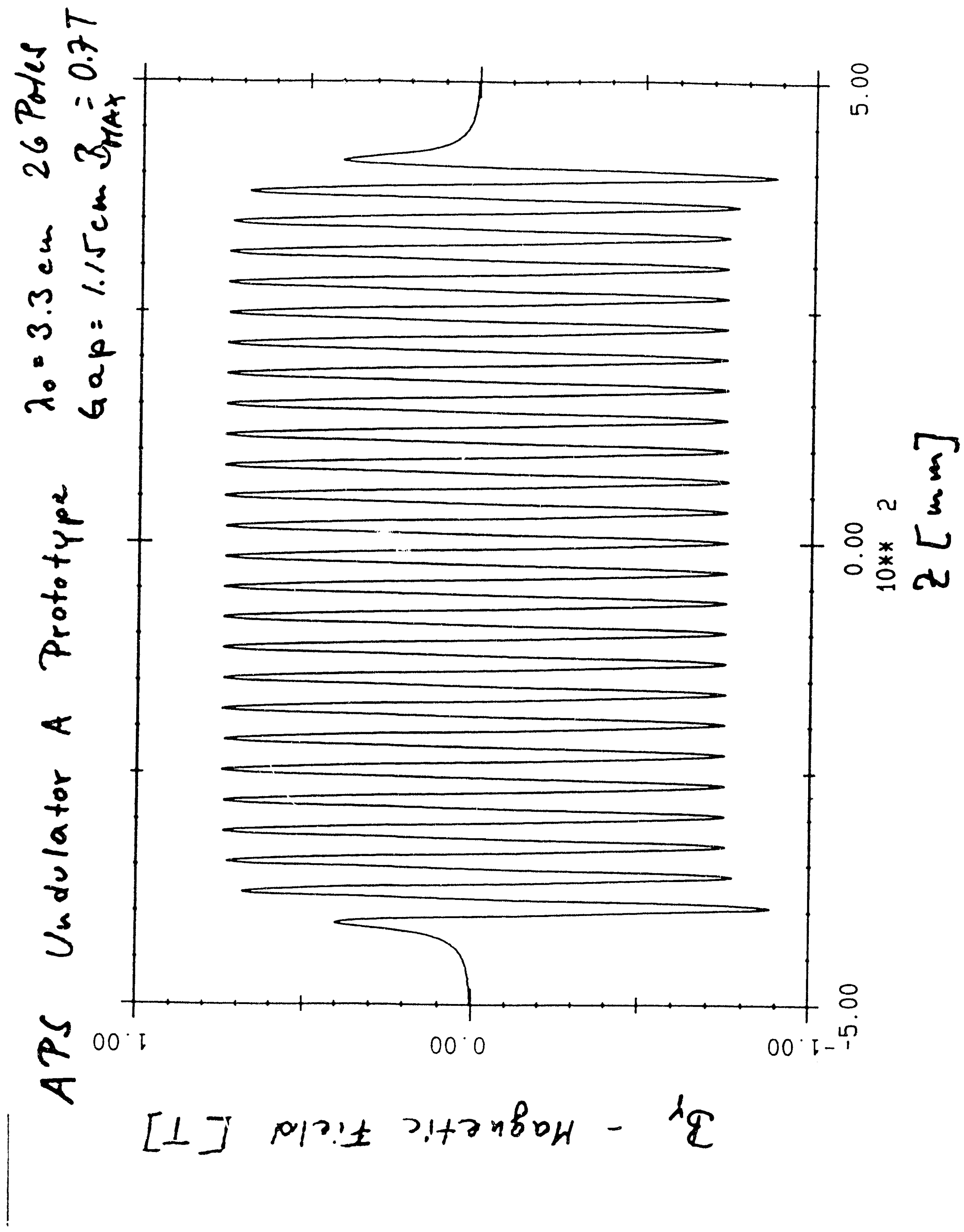
Precision Measurement of Multipoles

Data Processing

ALS Hassenzahl, Kincaid, Bahrdt package

HASYLAB

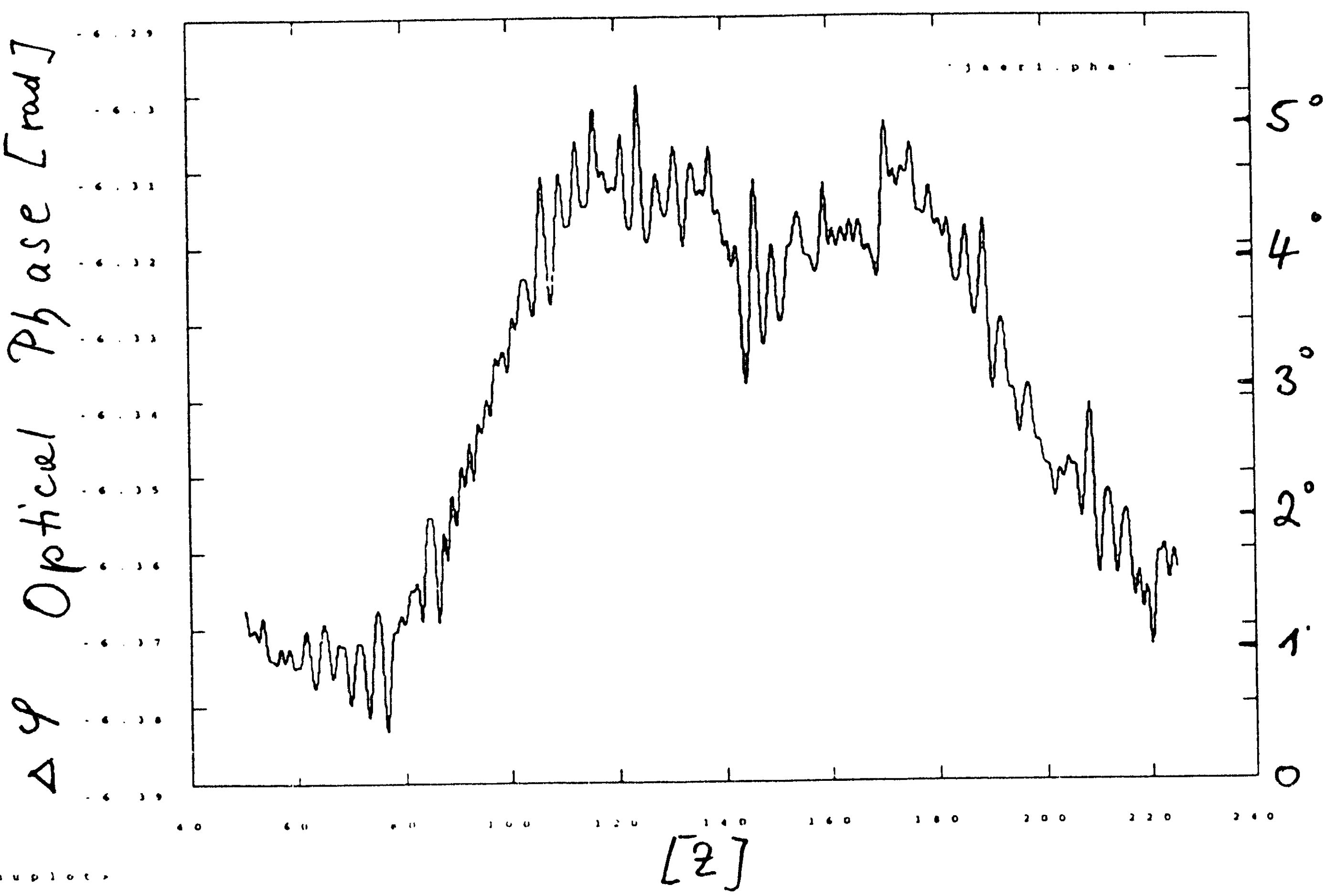

CAUTION
CAUTION



APS Undulator A Prototype
λo = 3.3 cm 26 Poles
Gap: 1.15cm B_MAX = 0.7T
By - Magnetic Field [T]
1.00
0.00
-1.00
-5.00
0.00
5.00
10** 2
Z [mm]

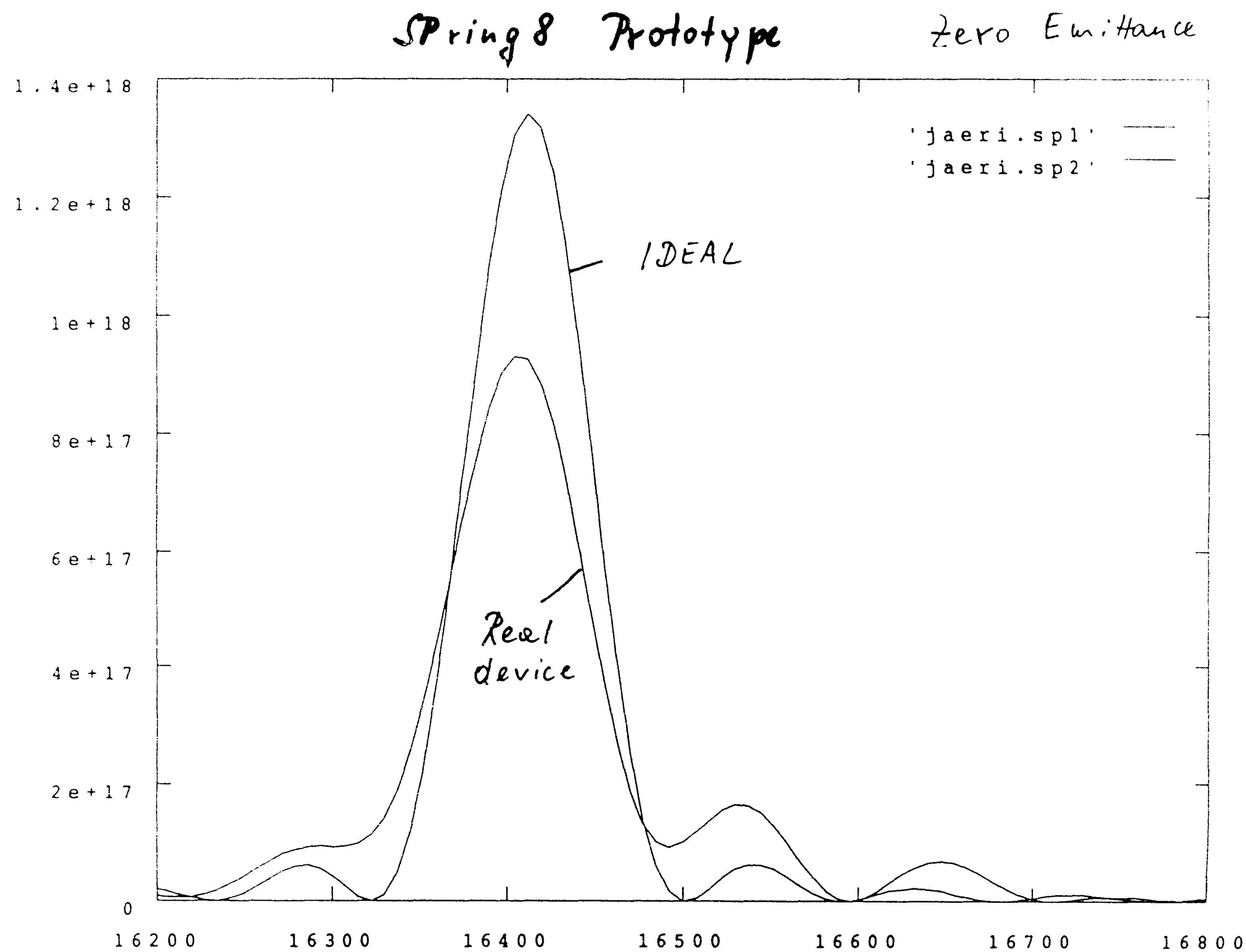
Spring 8 Prototype

$\lambda_0 = 3.3$ cm



Optical Phase change in the periodic part of the field

Unit is 2π (or 360°)

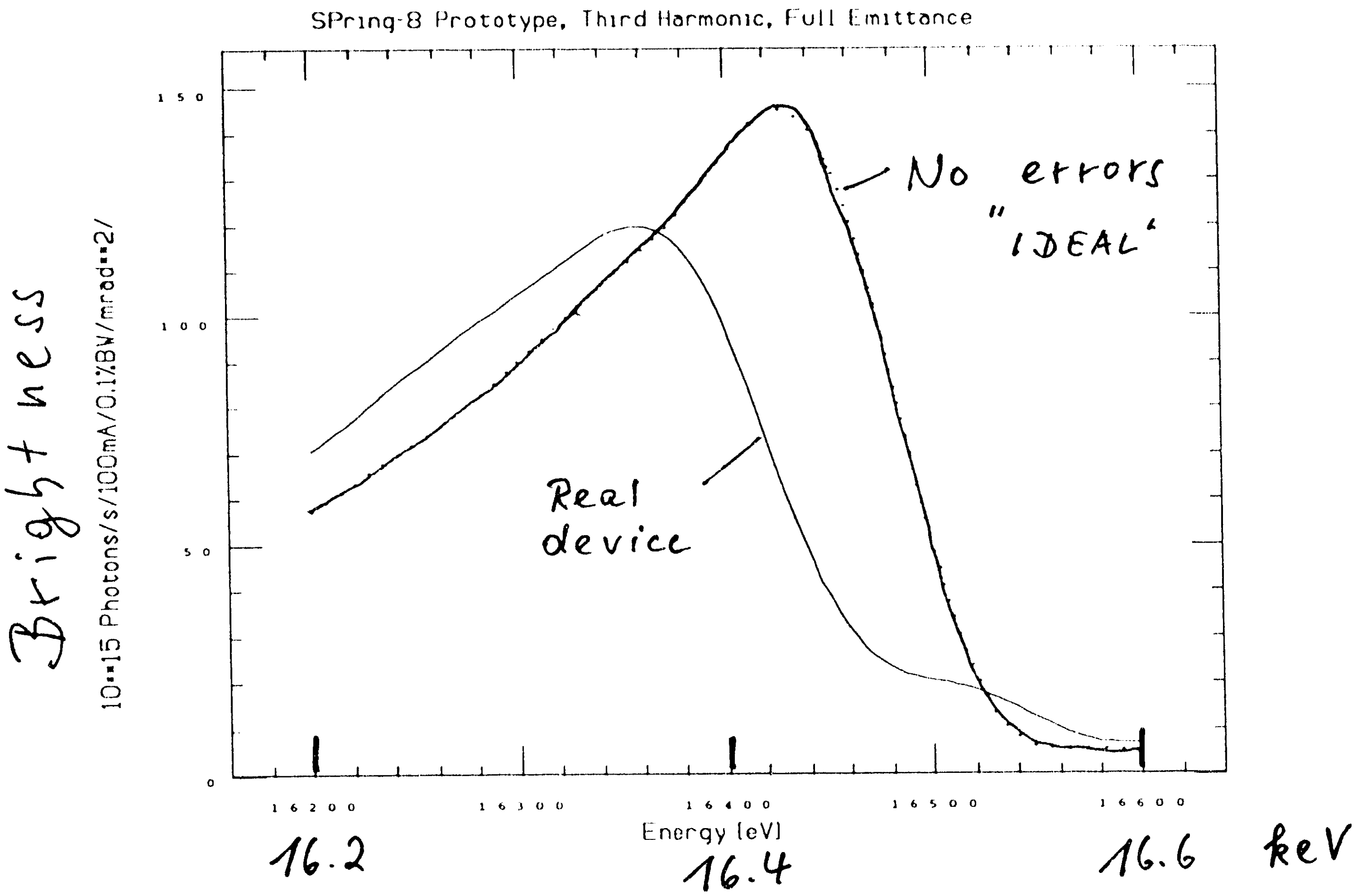

SPring8 Prototype
Zero Emittance
'jaeri.sp1'
'jaeri.sp2'
IDEAL
Real
device
1.4e+18
1.2e+18
1e+18
8e+17
6e+17
4e+17
2e+17
0
16200
16300
16400
16500
16600
16700
16800

gnuplot>

SPring 8 Prototype at APS

$\lambda_0 = 3.3$ cm

APS Emittance



Introduction to the User Technical Interface Group

Steve Davey

APS Fifth Users Meeting

October 15,1992

User Technical Interface Group

Program Goals

- Provide a seamless technical interface between the APS users and the APS facility. The group will provide a point of contact for technical issues between the APS and the APS users.
- Facilitate the integration of the user technical requirements with the APS activities.
- Coordinate the oversight of user beamline technical activities from conceptual design through commissioning.

User Technical Interface Group

Program Activities

- Assess user technical needs of each CAT
- Facilitate activities within the APS/XFD to address APS user needs
- Enhance technical documentation and information exchange
- Assure APS technical developments are included in beamline designs
- Coordinate beamline design reviews
  - -conceptual design in progress
  - -predesign
  - -engineering/safety design
- Ensure the quality and suitability of user support

User Technical Interface Group

Activities for the Next 6 Months

1. CATs beamline conceptual design reviews
   Design of 5 CAT beamlines were reviewed September '92
   Design of 10 CAT will be reviewed December '92

2. Use input from the CAT's conceptual designs to develop standard beamline components.

3. Provide guidance on the beamline pre-design requirements to all the CATs

4. Issue documents to specify beamline UHV standards and shielding requirements

5. Issue an updated document on the radiation characteristics of the APS

User Technical Interface Group

1993 APS/XFD Workshops

1. Standard Components Workshop
   February 1993

2. International ID Magnetic Measurement Workshop
   Spring 1993

3. X-ray Mirrors Workshop
   Summer 1993

User Technical Interface Group Example of the Integration of User Requirement

Design of laboratory for the production and characterization of x-ray optics.
CAT input was obtained to ensure that the user community needs were best filled.

The process:

1. APS proposed a design of the facility
   - -surface metrology laboratory
   - -mirror coating facility
   - -x-ray crystal optic fabrication facility
   - -x-ray characterization laboratory

2. User's needs were assessed
   - - *X-ray Optics Fabrication and Characterization Questionnaire* (7/92)
   - - *APS CATs Mirror Survey* (7/92)

The planned facilities were described, and specific recommendations were asked for the facilities, techniques, and equipment.

3. User's needs were integrated into the facility design.

User Technical Interface Group

Typical Activity: Diffractometer Standardization

To facilitate the development and standardization of the next generation of diffractometer software and hardware.

The APS is investigating integration of APS controls group EPICS software with standard diffraction software.

-A basic laboratory setup is in the process of being brought up in an EPICS environment.

-SUPER is being ported to EPICS.

Participation in the Computer Advisory Committee that was formed by the APSUO.

An APS users survey will be conducted to assess the user's diffractometer needs and to solicit recommendations for improvements.

User Technical Interface Group

e-mail

- scd@anlaps
- scd@anlaps.aps.anl.gov

User Technical Interface Group

Evolution of Activities

Near term (design phase):

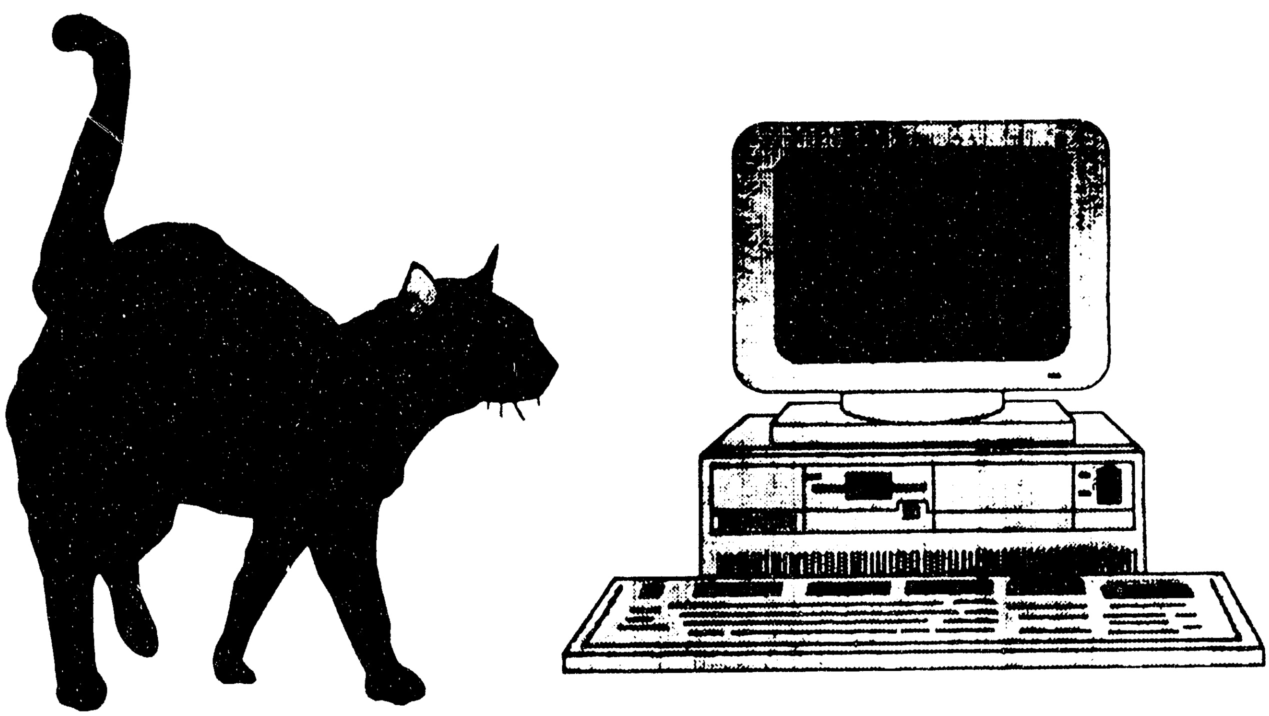
- Provide a technical point of contact, assess APS users technical needs, and assure the highest level of user technical communication and support.
- Coordinate detailed reviews of all the user beamline designs, from concept to final construction in order to assure construction of the highest quality beamlines.
- Ensure that user input is incorporated into APS/XFD designs and
Ensure APS technical developments are incorporated into beamline designs

Long term (operational phase):

- Provide the users with technical interface during commissioning and operations.
Continue to provide a technical point of contact.

ADVANCED NETWORKING AND DATA SYSTEMS IDEAS FOR CATS

Rick Stevens
Mathematics and Computer Science Division
Argonne National Laboratory
Argonne, IL 60439



This work was supported by the Applied Mathematical Sciences subprogram of the Office of Energy Research, U.S. Department of Energy, under Contract W-31-109-Eng-38.

Advanced Networking and Data Systems Ideas for CATs

- survey of new networking and data systems components
- PURPOSE: generate some new ideas for experimental area computing and networking
- foster joint planning of requirements and capabilities
- improve the effectiveness of the APS beamline computing systems
- reduce surprises on both sides

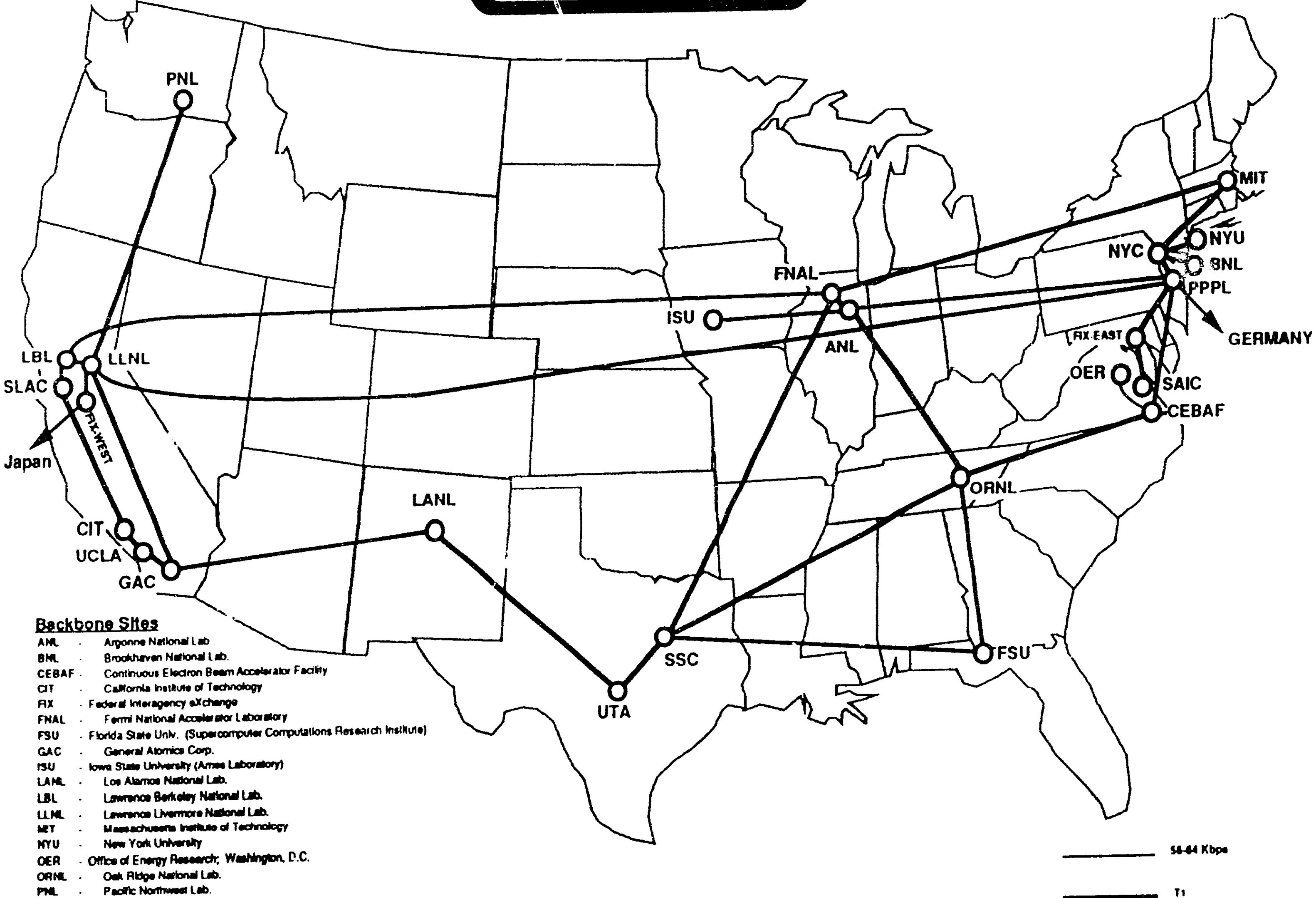
Outline of Topics to be Covered

- campus, regional and national networking connectivity
- new networking technologies
- networking alternatives
- new data system technologies
- prototypical data system configurations
- ANL high performance computing facilities planning
- remote interaction with experimental facilities
- invitation to collaborate (possible topics)

Campus, Regional and National Networking Connectivity

- structure of the NREN
- local connection responsibility of institution and regional networking consortium
- industry is welcome to join the regional consortia
- backbones will be provided by Federal $$$
- regional nets funded by variety of sources
- Gigabit testbeds are leading the way

ESnet Backbone 1991

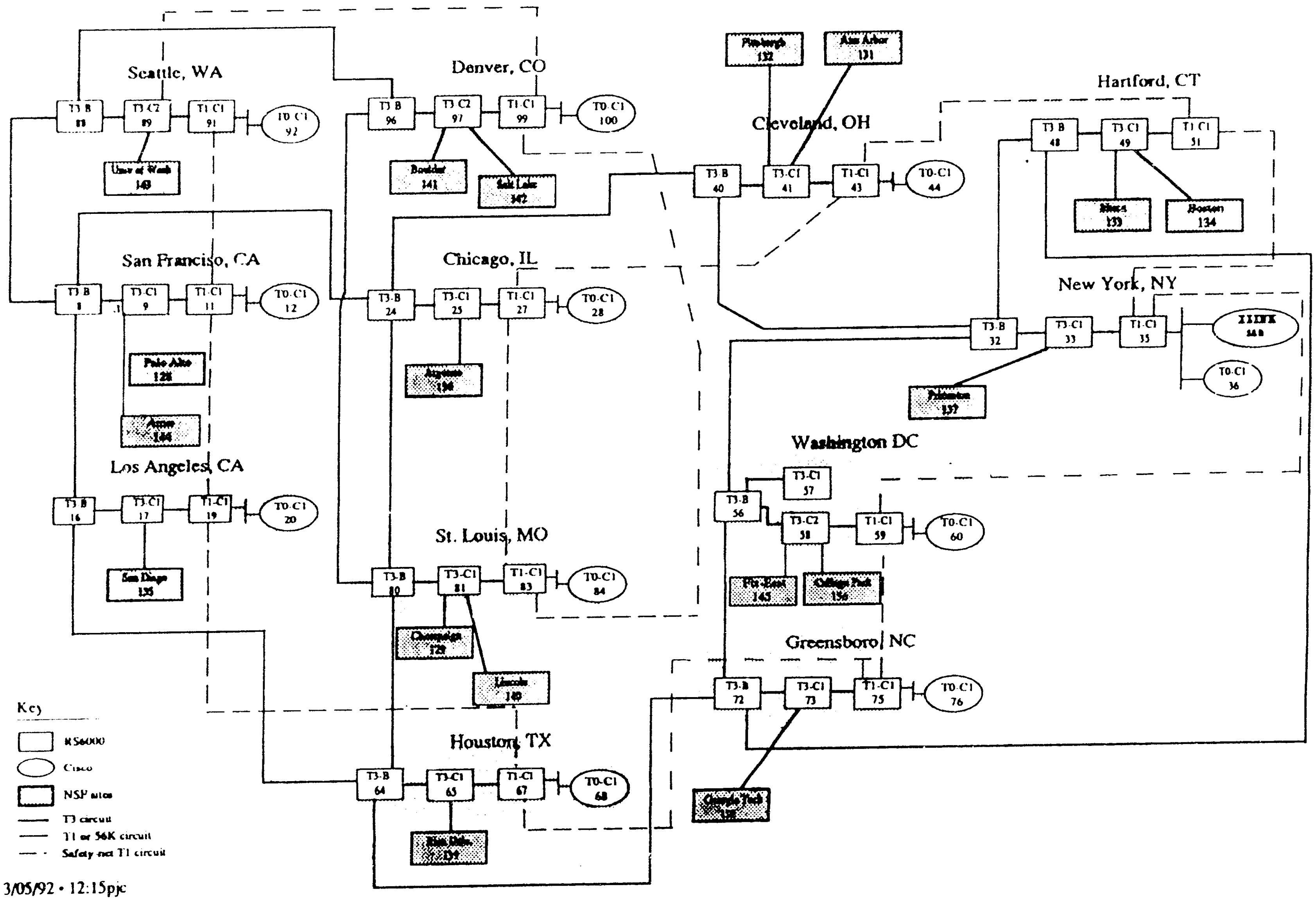


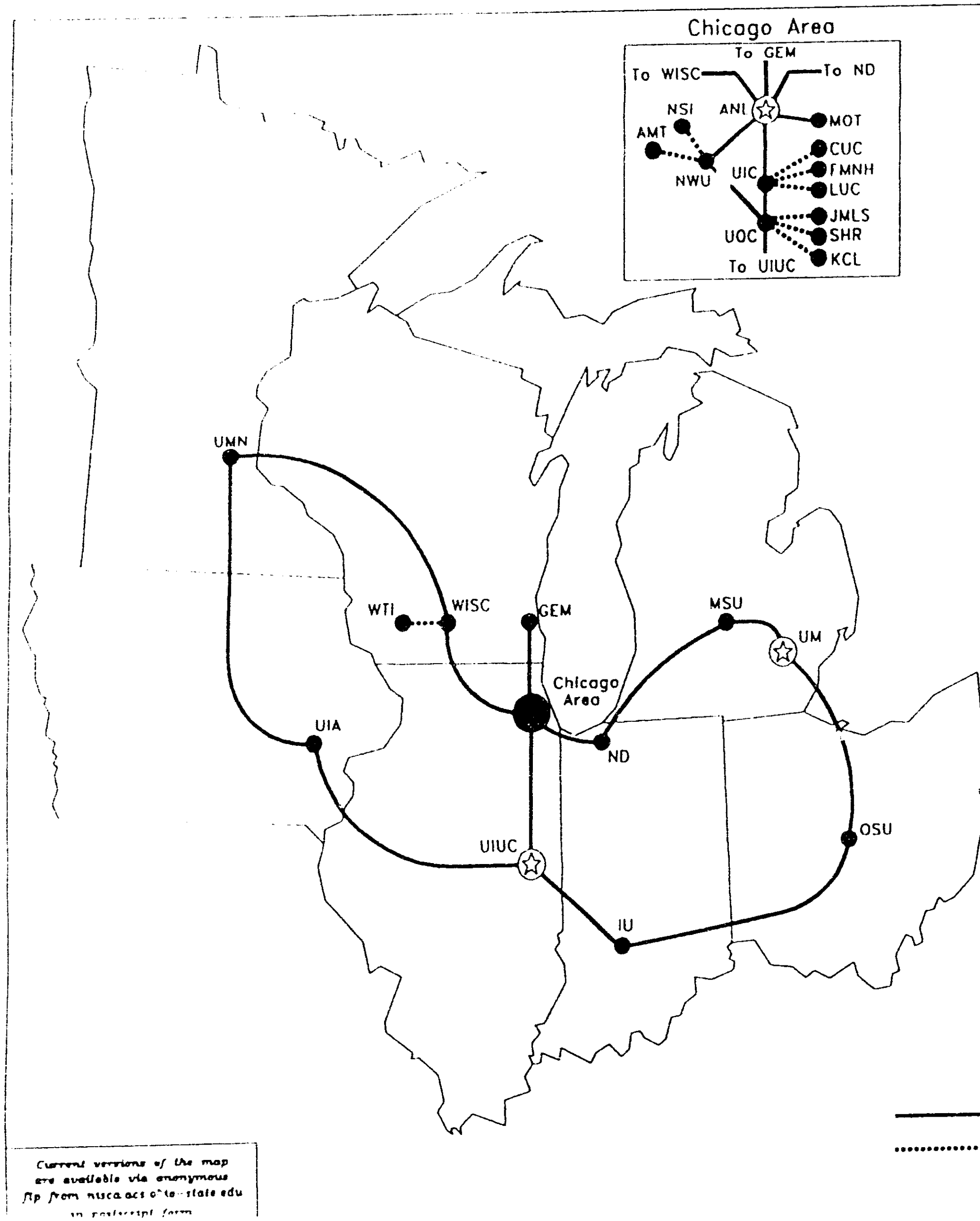
Backbone Sites

ANL - Argonne National Lab
BNL - Brookhaven National Lab.
CEBAF - Continuous Electron Beam Accelerator Facility
CIT - California Institute of Technology
FIX - Federal Interagency eXchange
FNAL - Fermi National Accelerator Laboratory
FSU - Florida State Univ. (Supercomputer Computations Research Institute)
GAC - General Atomics Corp.
ISU - Iowa State University (Ames Laboratory)
LANL - Los Alamos National Lab.
LBL - Lawrence Berkeley National Lab.
LLNL - Lawrence Livermore National Lab.
MIT - Massachusetts Institute of Technology
NYU - New York University
OER - Office of Energy Research; Washington, D.C.
ORNL - Oak Ridge National Lab.
PNL - Pacific Northwest Lab.
PPPL - Princeton Plasma Physics Lab.
SLAC - Stanford Linear Accelerator Lab.
SSC - Superconducting Super Collider
UCLA - Univ. of California, Los Angeles
UTA - Univ. of Texas, Austin (Fusion Research Center)

12 Oct 90

ANSNET/NSFNET T3 topolog:





CICNet

Logical Network Topology

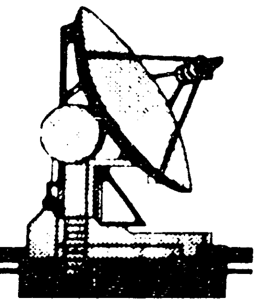
AMT = Ameritech Information Services Inc.
ANL = Argonne National Lab
CUC = Concordia College Chicago
FMNH = Field Museum of Natural History
GEM = GE Medical Systems
IU = Indiana University
JMLS = John Marshall Law School
KCL = Kent College of Law
LUC = Loyola University Chicago
MSU = Michigan State University
MOT = Motorola Inc.
ND = University of Notre Dame
NSI = Notis Systems Inc.
NWU = Northwestern University
OSU = The Ohio State University
SHR = SHARE Inc.
UIA = University of Iowa
UIC = University of Illinois at Chicago
UIUC = University of Illinois at Urbana Champaign
UM = University of Michigan
UMN = University of Minnesota
UOC = University of Chicago
WISC = University of Wisconsin
WTI = Wingra Technologies Inc.

* Indicates site is to be connected
☆ Indicates NSF backbone connected site

——— 1.5 Mbps
········· 56 Kbps

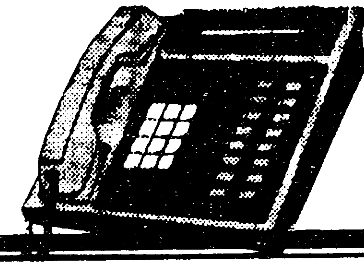
The Ohio State University
Academic Computing Services
Network Engineering Group
created on 1/21/91 by wjm+@osu.edu
revised on 9/30/92 by wjm

High-Performance Networks



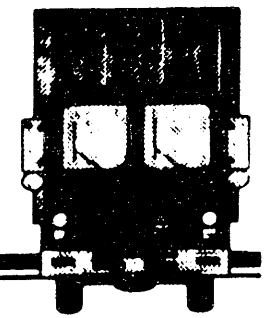
- WAN
  - NREN based on T3 (45Mbits) in 1992/3
  - NREN based on OC-48 (800 Mbits) in 1994/5
  - NREN = NSFnet + ESnet + NASAnet + MILnet + <regional internets>
  - CICnet (midwest internet consortium)
- LAN
  - FDDI backbone at ANL in 1992/3
  - HIPPI/FCS/SHIPPI backbone in 1994/5
- subLAN
  - *multiple HIPPI*
  - BUS based interconnects
  - optical freespace interconnects

ANL Onsite Networking Infrastructure



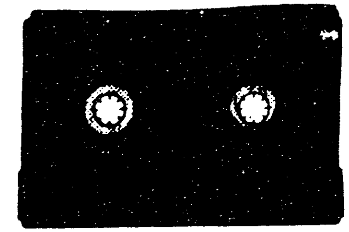
- labwide FDDI infrastructure in place 1992/3
- MCS testing of CDDI, FCS and HIPPI 1992/4
- APS should have multiple fibers to building 221
- FCS and HIPPI extender tests possible in 1993
- 100x FCS connections to B221 1995/6
- NREN and CICnet connections to B221

Networking Alternatives or Offsite Data "transport"



- data can be moved via networks or removable media
- FedexNET (using overnight mail to ship 8mm or DAT tapes), can move 5-1000 Gbytes in 24 hours at a cost of $1600 Media + $100 day
- Single T3 line can move 400 GBs in 24 hours (cost varies by distance)
- Single OC-48 line can move 8.6 TBs in 24 hours (cost >10x T3)
- initially it might be more cost effect for data movement to use FedexNET
- HOWEVER by 1996 moving the data should not be a problem, only storing and processing it

Data System Example Configurations

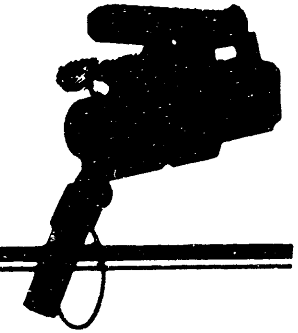


- consumer technology 8mm tape robot
  - 50 Gbyte capacity, 500KB/s transfer rate
  - < 5 minute search speed per 5 Gbytes
  - $10,000
- broadcast technology 19mm tape robot
  - 10 Tbyte capacity, 25MB/s transfer rate
  - < 5 minute search speed per 100 Gbytes
  - $500,000
- optical tape technology
  - 100 Tbyte capacity, 5 MB/s transfer rate
  - < 5 minute search per 1000 Gbytes
  - $200,000

Remote Interaction with Experimental Facilities

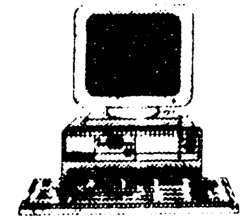
- Problem: beam time available 24 hrs/day, postdoc time 24 hrs/day but PI time 1 hour/day at remote site
- Desire: Increase the PI effectiveness by allowing him/her to interact with the experiment crew on demand from multiple remote location(s)
- Solution: *Telepresence*
- Short Term : interactive voice, video and computer ties to the experimental control area.
- Future: Virtual Reality interaction with experimental crew (stereo robot vision) etc.
- need to plan for networking requirements

Experiment Monitoring and Video Teleconferencing



- simple things that can be done for little $$$
- shared realtime computer window systems coupled to instrument controls, doable now if X windows or NeXTStep based
- modern instrumentation environment leverages multimedia PC/Workstation investments
- off the shelf ISDN /Internet based Video Tel Con Systems, require 64Kbps lines
- PC/Workstation based 6 person VTC systems for < $10,000
- multiplexed AD/DA control lines over internet/leased lines

Downsizing and Distributed Computing



- by 1995/6 the high-end scientific workstation will be capable of > 1 Gflops performance and will have a basic network interface of 10-100 MB/s ($20,000)
- PC class machines will have 100 Mflops and reasonable 10 MB/s network interconnect ($5,000)
- FCS switches and interface cards will enable flexible distributed computing environments
- postpone data acquisition and analysis HW decisions as long as possible

Invitation to Collaborate

- interested CATs are invited to have further discussions to investigate possible collaborative projects to develop the needed networking and data systems infrastructure

BUSINESS MEETING OF THE ADVANCED PHOTON SOURCE USERS ORGANIZATION

Roy Clarke called the Business Meeting of the APSUO to order on October 25, 1992. He congratulated Steve Durbin, outgoing Chairman of the APSUO Steering Committee, on a job done well for the past 18 months. He pointed out that Steve was instrumental in

- representing the users in Washington to help get APS "on the road,"
- working to promote the formation of the CAT Research Directorate, and
- presenting user needs to the APS.

In brief remarks, Steve Durbin indicated that the users organization is perceived to be the genuine voice of the users on the various issues that arise with respect to the APS. He mentioned that the APSUO Steering Committee was often called upon to represent the users at various hearings (DOE and Congressional) and emphasized that steering committee testimony is taken very seriously.

The gavel was then passed to Roy Clarke, new APSUO Chairman, who presided over the election of new Steering Committee members. He described the Steering Committee as an advisory body to the Associate Laboratory Director for the APS and an advocacy voice for the APS. Twelve candidates had been slated in advance by the Nominating Committee. No one was nominated from the floor. Users were asked to vote for up to six new members by ranking them in order of preference. The winning candidates — Michael Bedzyk, George Brown, Kevin D'Amico, Mark Rivers, Ian Robinson, and Heinz Robota — assumed office immediately after the end of the Business Meeting.

Following the annoucement of the election results, Roy Clarke closed the APSUO Business Meeting.

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PROGRAM

FIFTH USERS MEETING
for the
Advanced Photon Source

October 13-15, 1992
Argonne National Laboratory
Argonne, Illinois 60439
Bldg. 362 Auditorium

Tuesday, October 13, 1992

6:00-8:00 p.m.	**Registration - Holiday Inn of Willowbrook**

Wednesday, October 14, 1992

7:30-8:30 a.m.	**Registration - Bldg. 362 Lobby**

Morning Session: Advanced Photon Source: A Look Ahead (Stephen M. Durbin, Chair)

8:30 a.m. *Welcoming Remarks*
Alan Schriesheim, Director, Argonne National Laboratory

9:00 a.m. *Advanced Photon Source Project Overview*
David Moncton, Associate Laboratory Director for the APS

10:00 a.m. **Break**

10:30 a.m. *Beamline Funding: Opportunities and Mechanisms*
- DOE/BES -Bill Oosterhuis
- DOE/OHER - Roland Hirsch
- NIH - Charles Coulter
- NSF - Adriaan de Graaf

12:00 noon **No-Host Lunch (Argonne cafeteria)**

***Afternoon Session:* Advances in Synchrotron Radiation Applications (Alan Goldman Chair)**

1:30 p.m.	*Using High-Intensity X-rays at CHESS to Visualize How Polymerases Copy Genetic Material: 3-D Structure of HIV-1 Reverse Transcriptase Complexed with Double-Stranded DNA* Edward Arnold, Rutgers University *Powder Diffraction with Synchrotron Radiation* Anthony K. Cheetham, University of California, Santa Barbara *DAFS: A New X-ray Structural Technique Using Real Photons and Virtual Photoelectrons* Larry Sorensen, University of Washington *Coherent X-ray Optics: Soft X-ray Microscopes and Making Things Harder* Chris J. Jacobsen, SUNY, Stony Brook *Using Coherent X-rays for Scattering at the APS* G. Brian Stephenson, IBM
3:30 p.m.	**Tours**
6:00 p.m.	**Buses Leave for the Shedd Aquarium**
7:00 p.m.	**Reception and Banquet at the Shedd Aquarium**

Thursday, October 15, 1992

***Morning Session:* Advanced Photon Source: Technical Developments (Roy Clarke, Chair)**

8:30 a.m.	**APSUO Business Meeting**
9:00 a.m.	*"Top Off" - A New Operational Mode for the APS* John Galayda
9:25 a.m.	Developments in High Heat Load Optics Dennis M. Mills
9:50 a.m.	*Capabilities of the Storage Ring to Deliver Stable Photon Beams* Glenn A. Decker

10:15 a.m.	**Break**
10:45 a.m.	*Developments in Photon Beam Position Monitors* Tuncer Kuzay
11:05 a.m.	*Magnetic Measurements and Undulator Performance* Joachim Pflüger
11:30 a.m.	*APS User Technical Interface Activities* Steven Davey
11:50 a.m.	*Advanced Networking and Data Systems for Support Beamline Experiments* Rick L. Stevens
12:15 p.m.	**Election Results and Concluding Remarks**
12:30	**Adjourn**

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Philip Coppens (SUNY/Buffalo)
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Alan Goldman (Iowa State Univ./Ames Lab.)
Gene Ice (ORNL)
Samuel Krinsky (NSLS)
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Paul Sigler (Yale Univ.)
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Albert Thompson (LBL)
Keith Watenpaugh (Upjohn)

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