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ARGONNE NATIONAL LABORATORY
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Argonne, Illinois 60439

ANL/APS-CP-2

PROCEEDINGS OF THE SECOND USERS MEETING FOR THE ADVANCED PHOTON SOURCE

Held at Argonne National Laboratory
March 9-10, 1988

Advanced Photon Source Division

November 1988

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MASTER

FOREWORD

The Second Users Meeting for the Advanced Photon Source, organized by the Advanced Photon Source Users Organization (APSUO), was held at Argonne National Laboratory on March 9-10, 1988. Some 300 scientists and engineers from around the United States and from overseas took part. The principal reasons for the meeting were to celebrate the inclusion of construction funding for the APS in the President's January 1988 budget message to Congress; to remind the user community that their continued active support is required; and to begin organizing user groups and to make plans for building beam lines and other technical facilities for research.

Presentations included an overview of the APS project plans and status, accelerator design, insertion-device and beam-line plans, x-ray scattering studies, x-ray microtomography, studies of novel materials, time-resolved studies, and summaries of APS-related topical workshops. Participants toured a full-scale mock-up of an APS storage-ring sector. At the banquet at the Chicago Museum of Science and Industry, Kazutake Kohra, founder of the Photon Factory, spoke of plans to build a number of large and small synchrotron-radiation facilities in Japan.

High attendance at the meeting reflects continuing enthusiasm for the APS project among potential users. The meeting documented progress among users in forming topical subgroups to address specific research concerns and in considering issues of user access to APS beam lines. Users also adopted proposed bylaws for the APSUO and elected a new member to the organization's Steering Committee.

Conference Co-Chairs: David W. Lynch, Iowa State Univ., Ames Laboratory
Paul M. Horn, IBM, T.J. Watson Lab.

APSUO Steering Committee: Walter Trela, Los Alamos National Lab., Chair
Paul M. Horn, IBM, T.J. Watson Lab., Vice-Chair

Boris Batterman, Cornell Univ.
Arthur Bienenstock, SSRL
Robert Broach, Allied Signal
Katherine Cantwell, SSRL
Roy Clarke, Univ. of Mich.
Jerome Cohen, Northwestern Univ.
Peter Eisenberger, Exxon
Keith Hodgson, Stanford Univ.
Michael Knotek, NSLS
David Lynch, Iowa State Univ., Ames Lab.
Denis McWhan, Bell Laboratories
Keith Moffat, Cornell Univ.
R. Siemann, Cornell Univ.
J.H. Weaver, Univ. of Minn.

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PREFACE

This report documents the second Advanced Photon Source users' meeting. Since the first users' meeting 16 months ago, there has been increased interest on the part of the user community in the project and increased development of the project itself. This development has taken place not only as a result of much hard work by a strongly motivated group at Argonne, but also through the efforts of scientists at other laboratories, notably CHESS, NSLS, and SSRL, who have carried out research on concepts and components critical to the operation of the Advanced Photon Source. These are summarized at the end of this report.

A major part of these proceedings is an update on the facility itself. During the interval between users' meetings, a number of design improvements were made--some at the suggestion of the user community, some by other advisory committees, and some by the APS staff. More improvements may be expected in the future. One purpose of users' meetings is to inform prospective users about the facility and to introduce them to the personnel responsible for each aspect of its design and construction so that they may better interact with them.

A second purpose of users' meetings at this early stage is to bring users together so that they may discuss the formation of groups to build beam lines, influence the beam lines to be built by others, or do collaborative research on facility beam lines. The method of allotting beam lines and funds to build them has not yet completed its evolution. Considerable discussion of this issue took place at the meeting, and the public portions of this discussion are described in these proceedings. Private discussions should continue until user policy is settled. Suggestions from users are most welcome.

This meeting was relatively easy for us to organize, for there had been a number of workshops on topics of direct concern to the Advanced Photon Source, and summaries of those workshops were in order. In addition, some very fine research using x-rays had been done in the past year or so, and reports on some of this research formed a major part of the meeting. The harder part of the organization was the logistics, and these were taken care of in exemplary fashion by staff at Argonne. We especially wish to thank Bonnie Meyer.

David W. Lynch
Paul M. Horn

PROCEEDINGS OF THE
SECOND USERS MEETING FOR THE
ADVANCED PHOTON SOURCE

ABSTRACT

The second national users meeting for the Advanced Photon Source (APS) at Argonne National Laboratory -- held March 9-10, 1988, at Argonne -- brought scientists and engineers from industry, universities, and national laboratories together to review the status of the facility and expectations for its use. Presented papers and status reports in these proceedings include the current status of the APS with respect to accelerator systems, experimental facilities, and conventional facilities; scientific papers on frontiers in synchrotron applications; summaries of reports on workshops held by users in certain topical groups; reports on research and development activities in support of the APS at other synchrotron facilities; and notes from a discussion of APS user access policy. In addition, actions taken by the APS Users Organization and its Executive Committee are documented in this report.

WELCOMING REMARKS

Welcoming Remarks

Alan Schriesheim, Director
Argonne National Laboratory

Ladies and gentlemen, to tell you I am pleased to welcome you to this conference would be a gross understatement. I am purely delighted to meet with you and celebrate a landmark event -- the specific mention of construction funding in 1989 for the Advanced Photon Source in President Reagan's budget proposal to Congress.

During a gestation period of five years, the APS has passed other significant milestones. But none has been more important than the commitment to bricks and mortar that DOE and the President have now made and that I believe Congress will endorse. Each of you deserves praise for bringing along this vital project over past hurdles. It has taken your good work in science and engineering and your foresight in planning for the needs of the next century. It has taken your patience, your aggressiveness, and your judgment as to when to apply each of those techniques. Finally, it has taken the ability to swim strongly against a tide of tighter and tighter budgets in order to accomplish our mutual goal.

So I want to congratulate all of you and the broad array of institutions you represent. I especially want to acknowledge the presence and the contribution of Don Stevens, Associate Director of Basic Energy Science at the U.S. Department of Energy; George Duda of DOE's Office of Health and Environmental Research; Harlan Watson of the staff of the House Committee on Space, Science, and Technology; and John Straus, Executive Director of the Illinois State Governor's Commission on Science and Technology.

In addition, I can only broadly recognize the representatives present from a wide spectrum of industry -- ranging from coal to computers. And without the input and support of the university researchers, the APS might still be a gleam in the eye of a few scattered materials scientists. It took all this talent and more to bring us to our present happy state.

However, I do not want to sound as if this is the end of the race. As Churchill observed, this is not the end. It is not the beginning of the end. But it is the end of the beginning. Our reward for having done a good job to date is that we get to continue to do a good job in pressing this project forward to completion. We probably should consider ourselves halfway through the process. We started five years ago with the formation of the Eisenberger-Knotek Committee. God willing, we would like to complete the construction in something close to a like period into the future.

Our immediate goal is two-fold. First, we need to make sure that Congress supports the start of construction that has been proposed by President Reagan. It is essential that every member of Congress recognize the benefits that will be lost to our universities, to industry, and to American science generally if we delay this important project.

Our second immediate goal is to use the funding that has been provided to demonstrate top-level research management and leading-edge science and technology. This meeting is one of the essential means that we have of fulfilling that responsibility.

Finally, we have to keep a tight focus this year and in the years to come on the goals that we established for the Advanced Photon Source from the beginning of its planning:

- o We aim to make the APS the absolute forerunner in technology of its type in the world.

- o We expect the facility to generate first-class basic research in materials science.

- o And we are dedicated to making this the most user-friendly...researcher-convenient...cost-effective...user facility ever built in this nation.

I believe everyone in this auditorium shares those aspirations. When I consider the quality of the leadership we have drawn here today, I do not have the least doubt that we are going to achieve both our short-range and long-range goals. So at the same time that I welcome you, I want to thank you for the progress we have made in the past. Finally, I pledge to you Argonne's total dedication to realize the promise we all recognize in the Advanced Photon Source.

Thank you.

Introduction of U.S. Representative Harris Fawell

A key player for this project, as for any federally funded project, is the U.S. Congress. And a key congressional leader in representing the interests of the Advanced Photon Source has been our next speaker. He entered Congress in 1985 and immediately sought a seat on the Science, Space, and Technology Committee. There he holds an important post on the Energy Research and Development Subcommittee, which administers authorizing legislation involving the Advanced Photon Source. He has become an expert on the proposed facility and a reference source of information to his peers in Congress.

Please join me in welcoming a dedicated member of the APS Team... U.S. Representative Harris W. Fawell.

Introduction of APSUO Steering Committee Chair Walter Trela

As I said, we aim to make this the best user facility ever constructed. In addition to meetings like this, our primary source of guidance toward that goal comes from your Steering Committee. For the last year, the Chairman of that Committee has been a leader in the field, both as a scientist and as an organizer and administrator of research effort. We are fortunate to have in that position, and with us at this meeting... Dr. Walter Trela.

Welcoming Remarks

Congressman Harris Fawell
House Committee on Space, Science, and Technology

It is a pleasure to speak today before so many people interested in the Advanced Photon Source. It's also unusual, which is why you, as users, have an important part to play. I don't need to tell you how important this facility will be for scientific research and competitiveness. The presence of such a large number of potential users is proof of the importance of the Advanced Photon Source.

I would like to focus on the view from Congress. Last month we received the President's Fiscal 1989 budget, which calls for nearly a two-billion-dollar, or about 6%, increase for support of scientific research. That's good news. However, the last budget summit agreement allowed only a three-billion-dollar increase in all discretionary, nondefense spending. The fact that this increase comes primarily in the areas of science and technology demonstrates that the President is committed to improving the state of American research.

While I was delighted to see these numbers, I would be less than honest if I were to say that I expect Congress to agree to such a large increase in the science budget alone. Members of the House Science Committee, on which I serve, were decidedly skeptical when the President's Science Advisor, Dr. William Graham, testified on the science budget last month. The general feeling was that the other committees of the House would be unwilling to accept cuts in their programs in order to increase funding for science alone.

Needless to say, every program will be under intense scrutiny this year as we try to grapple with the deficits. Let me explain why I believe that, nevertheless, the Advanced Photon Source still has an excellent chance to receive the support it needs from Congress.

Competitiveness

First, the Advanced Photon Source is a machine for the times. Congress is awakening to the fact, as is the nation in general, that if we want to remain competitive in the global economy we need to invest in scientific and technological research. Clearly, the Advanced Photon Source is such an investment. You, the users, know how important materials research -- made possible by the APS -- will be for research and competitiveness. Industrial competitiveness makes a very compelling case for the APS.

National Project, National Constituency

Second -- and this is most important -- the Advanced Photon Source has a large and growing constituency. This is not just an "Argonne" project; nor is it an "Illinois" project: This is a national project, with a national constituency. You, the users, represent a diversity of industries, universities, and research institutions from across the country. Let me, as a member of Congress, emphasize to you that the greater the number of members of Congress who hear that they have a firm or university or research institution in their districts that is supportive of the Advanced Photon Source, the more we can count on their support. You have the interest, you have the understanding -- communicate that interest, that understanding!

Investment Quality

Third, the Advanced Photon Source will be a very good investment. The potential payoffs could run into billions of dollars in new technology to benefit the national economy. On the other hand, the costs are modest.

Of course, the shorter the construction period, the less the total cost. But even if the cost rose to half a billion dollars, it would represent less than one-third of one percent of the total federal nondefense research budget, given current levels. I feel confident my colleagues will recognize the soundness of this investment -- especially if reminded by their constituents.

Location

Finally, we could have found no better place to make this investment. Argonne National Laboratory has an excellent reputation for designing, constructing, and operating accelerator facilities. One need look no further than the Intense Pulsed Neutron Source and the ATLAS accelerator here at Argonne to know that this is true.

Relationship to Industry

In addition, Argonne is recognized as a good friend to industry and to scientists from outside the Laboratory. During Dr. Graham's appearance before the House Science Committee, he specifically complimented Argonne as the nation's leading laboratory in technology transfer and collaborative research with industry.

Welcoming Remarks

Donald K. Stevens, Associate Director for
Basic Energy Sciences, Office of Energy Research
U.S. Department of Energy

It is a pleasure to be here today. I sometimes wondered whether this pleasure would ever occur. I know that there are many in this audience who had those same concerns, whether we would ever reach a point where in fact this project was in the budget and before Congress for funding. I would like to add a couple of comments to those made by Congressman Fawell earlier. There are things to be done before we reach that final day when we will have an opening ceremony under way. And this audience here has a large part to play, in the immediate future and in the years to come.

Congressman Fawell mentioned that we have a very serious hurdle to get over yet, and that is the actions of Congress to authorize the project and to appropriate funds for the project. He pointed out that you people are particularly important in this phase when you talk to your Representatives back home and instill in them your enthusiasm for this project. I want to add, however, a note of warning. And that is, sometimes to do the job only half way can cause more problems in the end than if you don't do the job at all. It is one thing to get the Representatives to recognize and follow the importance of a given project, but there has to be a follow-up effort to make sure the funds are provided with it.

As an example that may be meaningful to you, there is a problem that we at BES Programs have this current fiscal year. There were a number of projects written into the program for BES, for which funds were provided, and these were construction projects for laboratories, university campuses, and so forth. You all heard about those things, I won't say any more about them. But in addition to that, there were a number of items earmarked in our operating budget. Funds were provided for some of these and not for others. For instance, the Materials Science program, which is the principal funding program for the Advanced Photon Source, had $27.7 million worth of research earmarked by Congress because of constituents who had gone to their Representatives to say "Hey, this is good stuff; make sure they do it." For $27.7 million in such earmarked research, they only provided an additional $2.7 million in our operating budget -- a $25 million shortfall, which has to be eaten by the program. Unfortunately, it is a wind-out budget -- that is, so much for materials and so much for chemistry, etc. -- and these things were earmarked for the materials program, so we can't steal from chemistry to help out on such a problem. I simply put this in front of you to warn you that you must do a complete job. It is an important job you must do. Please follow through and make sure it is done completely; otherwise, we get into trouble. Because then we might have to be in the position of stealing from SSRL or from NSLS or whatever for here; then we would really have an insurrection, and we wish to avoid that.

Another thing I would like to bring to your attention: names of people and groups that have been key players in bringing this project to its present state have been mentioned. One who hasn't been mentioned and who played a very critical role is Al Trivelpiece, Director of the Office of Energy Research. Al Trivelpiece was one of the best directors of the Office of Energy Research and its predecessor or organizations that we have in the scientific community have ever had the pleasure of having in such a position. He was a magnificent intellectual, knowledgeable person. He figured out how to get things done. You think back about four years ago and think about looking forward from that point. Al Trivelpiece had in front of him the big problems associated with funding projects in the magnetic energy fusion program. SSC was already on the track and moving. The Seitz-Eastman Committee had come forward with recommendations from the condensed-matter community to build a 1-2 GeV source with a $100 million pricetag on it, a 6-7 GeV light source with a $400 million pricetag, the Advanced Neutron Source with a $600 million pricetag, and the Relativistic Heavy Ion Collider with a pricetag somewhere in the $600 million range, along with CEBAF and a few others: an absolutely horrendous pie, if you will, that had to be cooked, baked, and separated out somehow. And after you people, the scientists, had convinced us that you needed these things, it was our job to convince Al Trivelpiece and the Department, to go to the OMB, to get it into the President's budget, to go to Congress, and for you again to get into the picture and convince your Representatives that this was the right thing to do.

A critical step at that time was to get it in the DOE budget as a logical thing for DOE to do. That was Al Trivelpiece's problem, and he did it, in a magnificent way. He took those four projects -- the 1-2 GeV source, the 7-GeV source, the Advanced Neutron Source, and the Relativistic Heavy Ion Collider -- as a program to revitalize the aging DOE laboratories. And it was specified then, the 1-GeV machine for Lawrence Berkeley Laboratory, the 7-GeV machine for Argonne National Laboratory, and this settled the half so there was going to be no more doubt on where things were going to be located. And the neutron source would clearly go to Oak Ridge National Laboratory, and the RHIC to Brookhaven National Laboratory. That plan went through with little or no debate. The Secretary of Energy bought it, the OMB bought it, and we were on the track. If he hadn't come up with that idea, we would still be fiddling around figuring how to get even one of these things in. I think, then, one has to remember Al Trivelpiece as playing a very critical role, a role that only Al could have swung in view of the high esteem in which he was held in Washington.

Well, so be it. Of those four, I am proud to say, two of them are on the road. The 1-2 GeV source, you know, is under construction out at Berkeley. We now have the 7-GeV source in the President's budget. We have high hopes for the Advanced Neutron Source in about 1991. The Relativistic Heavy Ion Collider is kind of shaky, but that is not a problem of mine. The big job is ahead. We got through the politics, at least in the Executive Department. We have to crash this final barrier in Congress, and then the heavy load and responsibilities on Argonne and its staff begin. They can do it, backed up by a user group, and we have here one of the strongest user groups I have seen. You have a continuing part to play after the authorization and the funding to express your wishes and see that the Laboratory produces what you need to do the best science for this nation and the world. Thank you.

Welcoming Remarks

Walter J. Trela
Los Alamos National Laboratory

On behalf of the Advanced Photon Source Users Organization Steering Committee, I too welcome you to this, the Second Users Meeting for the Advanced Photon Source. There are several reasons why we are having this meeting at this time. The first is that this is truly a time of celebration, and we will celebrate. We have been confident that our scientific and technical plans for the Advanced Photon Source would become reality. The appearance of the APS as a construction project in the President's Budget for FY1989 marks a major milestone toward achieving that reality and provides us with an occasion for celebration.

Through the efforts of dedicated individuals from Argonne National Laboratory, the University of Chicago, the Department of Energy, the Office of Management and Budget, the U.S. Congress and its staff, and the national synchrotron radiation user community, this tremendous success has been achieved. I want to thank all those responsible.

While we celebrate, we all should know that there is one final step required in the political process -- Congressional approval of the President's budget. Again, we are confident that we will succeed. Through many peer reviews, workshops, and this user community activity, the scientific and technical case for the APS has been made and verified. Congress knows of these justifications, and we believe that there is strong support for the APS in Congress. However, there also are very strong budget pressures, and we need to continue to articulate the scientific importance of this project so that it achieves final approval in the Congress. This is the second purpose of this meeting, to remind you that your continued active support is required.

A third reason for having this meeting now is to begin to organize user groups and to make technical, scientific, and financial plans for building beam lines and other technical facilities required to accomplish the research that we want to do with the APS. I would like to call to your attention the numerous sessions in this meeting that will help you to achieve these objectives. Beginning with Dave Moncton's talk and for the rest of the morning, you will hear a series of presentations from the Argonne staff describing the APS project, the accelerator, insertion devices, laboratory and support facilities, and so forth. This afternoon we have a session, "Frontier in Synchrotron Applications," that will highlight some of today's exciting research in the synchrotron radiation community. We hope this session will point toward some of the opportunities that will open up with the advent of the APS.

In order to stimulate specifically ideas for the future science that can be accomplished with APS, the APSUO Steering Committee has sponsored a series of workshops, the results of which will be reported on Thursday morning. The focus for user organization planning for the APS at this meeting is the User Subgroup meetings tomorrow. I urge you all to attend the meeting in your area of interest. Lest someone think it is too early for serious planning, we already have heard expressions of concern regarding some groups locking up certain funding sources.

Well, let me welcome you all again. I believe that this meeting will be an important step on the path toward the APS and the science that will follow.

Welcoming Remarks

John Straus, Executive Director
Governor's Commission on Science and Technology
State of Illinois

On behalf of Governor James R. Thompson I want to welcome you to Illinois and the Second APS User's Conference here at Argonne National Laboratory. And I want to thank you on behalf of the Governor's Commission on Science and Technology for this opportunity to address you this morning.

We are very fortunate in Illinois to be the home to Argonne National Laboratory. The Laboratory, as an international multi-purpose research and development facility, serves an important role in the state's economic development mission. State government is involved in supporting Argonne in areas which are beneficial to both the Laboratory and the State. Our efforts in this regard have taken many forms. For example, when the synchrotron is built, Illinois will pledge financial support to build housing for visitors to this state of the art facility.

Illinois recognizes Argonne's immense scientific and technical resources and since 1984 has supported the Laboratory's operation of a technology commercialization Center to develop, transfer, and commercialize new and advanced technologies. This Center, with funding from the state, works with Argonne personnel and Illinois businesses to identify new technologies that can be applied to the needs and wants of our businesses. Further, Argonne has received a $200,000 grant from the state to form the Illinois Superconductivity Institute, a multi-institution consortium, which will bring business and industry together with Argonne's staff to collaborate on applied research projects in superconductivity.

Argonne is also a key player in at least three other state-supported programs. The Midwest Plant Biotechnology Consortium, which was started here at Argonne, has received a $200,000 grant from Illinois in support of its efforts for the agricultural economy. Argonne and Illinois have also teamed with other institutions and a number of Illinois businesses, to form the Illinois Defense Technology Association, conceived to enhance Illinois' efforts to pursue federal research and development procurement opportunities. Illinois' relationship with Argonne National Laboratory is unique. No other state has developed such a strong partnership with a federal laboratory. Of this fact, we are perhaps most proud and most appreciative of Argonne's interest in Illinois, its businesses, and their economic development.

In closing let me thank you again for this opportunity to tell you a little more about Illinois' efforts to develop new technologies, and the important role Argonne plays in that plan. I welcome you again to our state, and wish you success at your research, and the best for a worthwhile and productive conference.

PRESENTATIONS BY APS STAFF

ADVANCED PHOTON SOURCE*

David E. Moncton, Acting Project Director
Advanced Photon Source

I would like to start by mentioning some things I think are important and probably unique about this project in the history of the field of synchrotron radiation. This project has some important strengths, the first of which is the very intense involvement by the user community. This project was a user-driven initiative, predating the interest of Argonne National Laboratory, and the users have been very actively involved. The APS Steering Committee and its subcommittees have worked closely with the project staff and made valuable contributions to the design.

This project and the ALS project at Lawrence Berkeley Laboratory, as the chief priorities of the laboratories at which they're sited, represent transitions in the history of synchrotron radiation. There is a very strong commitment by Argonne National Laboratory to this project. The project staff is dedicated to the job organizationally within the Laboratory, and it reports directly to the Director of the Laboratory, Dr. Schriesheim, and can draw on the Laboratory's resources very effectively.

And, of course, we have a strong belief in frequent external review. You can be sure that the cost, schedule, and technical basis for this project have been thoroughly reviewed by many different groups of experts.

We have estimated the total cost for the project at $274 million in FY 1987 dollars; this includes the conventional facilities, the technical components, and the beam lines. Contingency costs of around 25% of the total project are explicitly included, so the total cost in FY 1987 dollars is set at $336 million. Conventional facilities are the largest component at $110 million, followed by a contingency of $61 million and an estimated cost of $57 million for the storage ring.

Depending on the rate of funding, there are escalations that come into the final total cost. In the President's budget, $6 million is proposed for FY 1989, following on for a total of seven years, with commissioning in April 1995 and initial operations in April 1996 at a total cost of $456 million for construction. In our judgment, we could build the APS in five years on an optimal schedule of funding, with a completion date of April 1994. While we do understand the considerations that face both the Department of Energy and the Congress as they wrestle with priorities, we urge all of you to push the case, to the extent you can, for expeditious funding.

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*The summary presented here is based on notes taken at the meeting; copies of viewgraphs were provided by the speaker.

A number of things are going on at the site. The environmental assessment is an important preconstruction site-assessment effort, and a comprehensive environmental assessment document is very near completion. Another assessment activity has to do with cultural resources. The archaeologists have been out there for the last two years, and the field work is now completed and a summary report is being prepared. A final category of site-assessment activities, geotechnical studies, is very important to the project to certify that we will have a stable foundation for the buildings. The state has provided matching funds for a program involving the Illinois State Geological Survey.

Let's turn to the accelerator itself. We want to produce x-rays in the spectral range from 1 to 100 keV. We are designing this facility to have stored currents in excess of 100 mA. The emittance will be low, on the order of 10 nm-rad or less. The undulators should reach energies up to 20 keV, providing access to all the elements with K or L edges and all the energies important for x-ray diffraction. It would be appropriate to be able to tune the energy in each undulator over a wide spectral range: A group of scientists decided the most effective arrangement is to be able to tune the first harmonic from five to 15 keV and the third harmonic from about 15 to 40 keV. This tunability has been achieved by raising the circulating beam energy from 6 GeV to 7 GeV.

The storage ring design includes 40 straight sections, with 34 available for insertion devices. We expect to have 35 bending magnet sources, for a total of 69 sources. Some of these sources will feed multiple experimental stations, either by splitting a bending magnet beam or by using optics to deflect an undulator beam. So there could be on the order of 100 experimental stations around the ring.

There is a $40-million beam-line trust fund to be used to develop an optimal experimental program. The question is, how far will the $40 million go in instrumenting the facility? Roughly speaking, an undulator beam line outfitted with a reasonable selection of hardware will cost about $3.2 million; a shorter undulator, $2.9 million; a wiggler, $2.8 million; and a bending magnet line, $1.3 million. One strategy would be to build eight complete, project-funded beam lines for $20 million and fund insertion devices and front ends for access by various teams with the remaining $20 million. We expect to have those parts of the beam line that lie behind the shield wall funded by project funds, while collaborative teams build the parts outside the shield wall.

A subcommittee under the APSUO Steering Committee is to develop the policy for user access. At its first meeting, it was agreed a user policy would be set about a year from now. It is our thinking that each sector of the storage ring -- one insertion device and its accompanying bending magnet -- should be run by a collaborative team. Let me emphasize that independent investigators not associated with these teams would have access to nearly all the beam lines, because a fraction of time would be reserved on each of the beam lines. We want this facility to be as open as possible, but there has to be a commitment on the part of independent investigators, as well as the collaborative teams, and that commitment has to be assessed in some manner in allowing access to the facility.

ADVANCED PHOTON SOURCE

PROJECT OVERVIEW

Project Strengths:

- User Involvement in Design
- Institutional Commitment
- Dedicated Project Staff
- Frequent External Review

Project Highlights:

- User Activities and Reviews
- Project Cost and Schedule
- Site Assessment Work
- Accelerator Complex
- Conventional Facilities
- Beamline Facilities
- User Access Issues

WORKSHOPS AND CONFERENCES

October 1984	Ames Program Review
March 1985	Machine Physics Workshop
October 1985	Project Planning Workshop
December 1985	Scientific Case Workshop
December 1985	Insertion Device Workshop
May 1986	Ring Energy Task Group
November 1986	First Annual Users Meeting (300 Attendees)
November 1987	Joint X-ray and Neutron Scattering Workshop (3M Satellite Meeting)
November 1987	RF Workshop
December 1987	New Materials Workshop
January 1988	Geosciences Workshop
January 1988	Time Resolved Studies Workshop
January 1988	X-Ray Optics Study Group

Future Meetings:

February 1988	Industrial Applications Workshop
March 1988	Second APS Users Meeting
Summer 1988	Medical Imaging Workshop

REVIEWS

CDR-86

February 1986	Ad hoc Review, Lake Geneva
March 1986	ER Construction Readiness Review
April 1986	MA Validation Review

CDR-87

February 1987	APS Steering Committee Review (Accelerator System Conventional Construction R&D)
May 11, 1987	APS Steering Committee Review (Beamlines, Costs)
May 12, 1987	Independent Cost Estimate (ICE) Review
May 21, 1987	MA Validation Review
May 27-28, 1987	Accelerator Advisory Committee Review
June 9-11, 1987	ER Construction Readiness Review
June 1987	ICE Reconciliation
July 1987	APS Users Organization Subcommittee Review (Conventional Facilities)
September 1987	APS Steering Committee Meeting
October 1987	Accelerator Advisory Committee Review
November 1987	MA Validation Review (Conventional Facilities)
December 1987	APS Steering Committee Meeting

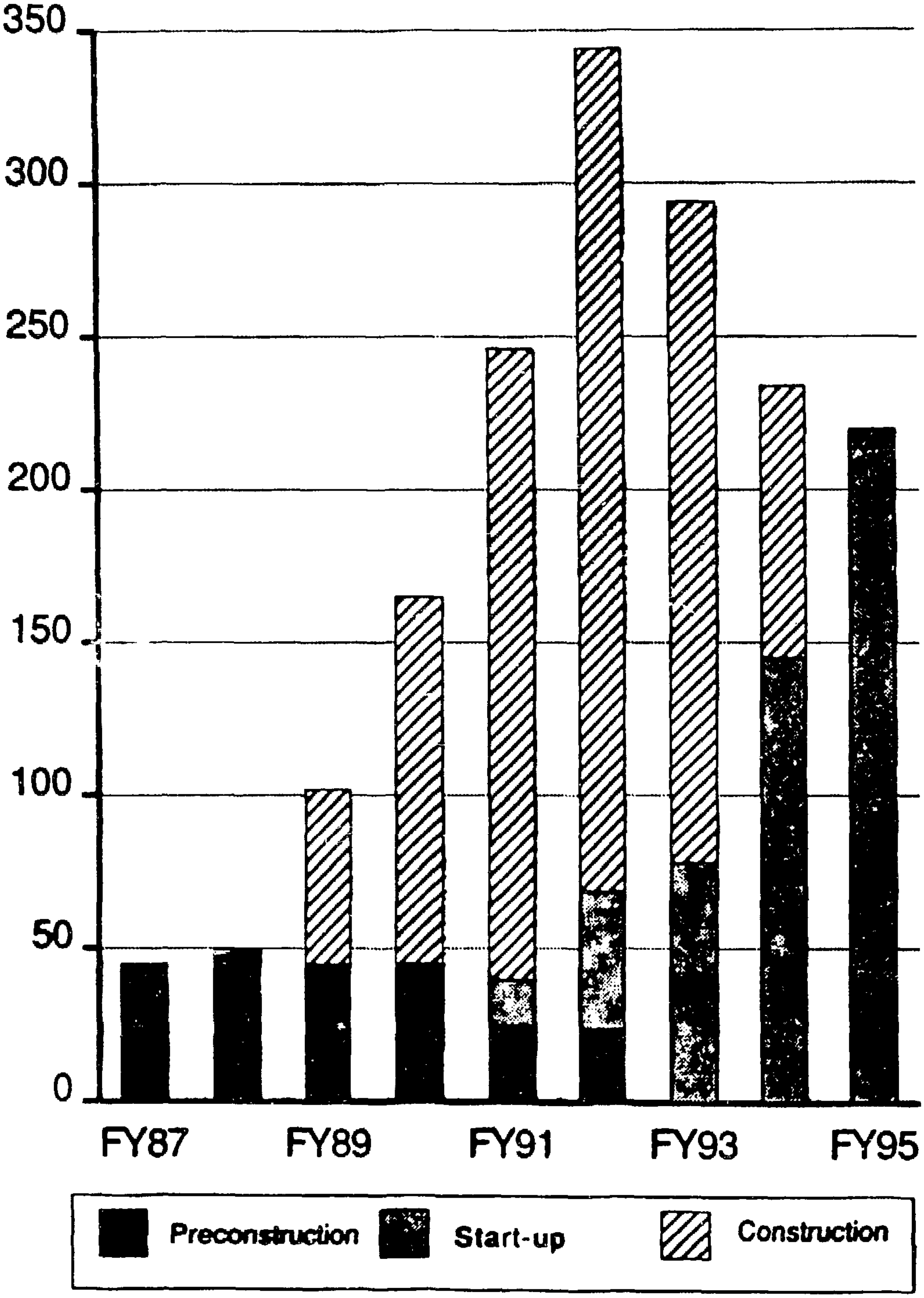
FY 87 DOLLARS:

Estimate	274.53
Contingency	61.61
Sum	336.134

Project Management	12.599
Injector	28.911
Storage Ring	57.148
Insertion Devices and Beam Lines	41.066
Computer Systems	8.712
Technical Component Support Facilities	5.007
Conventional Facilities	109.316
Miscellaneous Costs	11.767
Contingency	61.608

	FY89	FY90	FY91	FY92	FY93	FY94	FY95	FY96	TOTAL
PRESIDENT'S BUDGET								4/96	
(in $M)	6	39	68	90	92	111	45	5	456
ANL "OPTIMAL" COST SCHEDULE						4/94			
(in $M)	20	70	110	125	80	25	00	00	430

Effort Distribution



ADVANCED PHOTON SOURCE

SITE ASSESSMENT ACTIVITIES

Environmental Assessment

- U.S. Fish & Wildlife Service finds no endangered species problem.
- U.S. Army Corps of Engineers must issue permit to allow alteration of wetlands.
- Comprehensive Environmental Assessment by ORNL is near completion (expected April 1988).

Cultural Resources Survey

- Field work is completed.
- Evaluation of prehistoric sites (circa 6000 B.C.) shows subsurface features and artifacts related to butchering, cooking, hide preparation, and habitation.
- Historic sites (circa 1840) predate construction of the Illinois-Michigan Canal.
- Summary Report to be ready for the State Historical Preservation Officer (April 1988).

SITE ASSESSMENT ACTIVITIES
(Continued)

Geotechnical Studies

- The State of Illinois has provided $250K for the Illinois State Geological Survey to characterize subsurface soils and their stratigraphy.

- Current 24-hole drilling program and geophysical studies will provide the basis for foundation design and vibrational analyses.

USER GOALS

For Optimal Experimental Program

1. Beam Stability

   - Position and angle
   - Constant current (top-up mode)
   - Independent control of ID's
   - Reliability > 95%
   - Operations > 75%
   - No extended shut-downs

2. Conventional Facilities

   - Maximize access to BL
   - Provide adequate floor space
   - Provide convenient office/lab space
   - Support facilities, housing, etc.

3. Beamlines

- Provide a flexible radiation source
- Develop prototypes for optical components
- Make beamlines affordable
- Take advantage of "quantity production" without sacrificing capability
- Develop an appropriate "PRT" policy
- Provide "general user" facilities

BEAMLINE DEVELOPMENT PLAN

- $40M Beamline "Trust Fund" (Phase I)
- Beamline Planning Committee

Average Cost in K$ of Major Component Group for the IDs and Bending Magnet

Source	Source Cost	Front-End	Beam Transport First-Optics	Experimental Station	Total
Undulator (5m)	1326	487	476	1196	3495
Undulator (2.5m)	796	487	476	1196	2955
Wiggler	683	447	476	1196	2802
Bending Magnet	-	351	-	952	1303

USER ACCESS PROCESS

- APSUO Access Policy Subcommittee: March 1988
- Policy to be Set: April 1989
- Establish Review Committee: January 1990
- Access Approved: April 1990

USER ACCESS IDEAS

- Each sector (ID & BM) run by a collaborative team.

- Collaborative teams will be of various types. For example,

    * "Third party" national facilities, e.g., DOE/OHER proposed biomedical complex.

    * Universities.

    * National laboratories.

    * Industries.

    * Synchrotron service companies.

    * Argonne research divisions.

    * Advanced Photon Source

- Proposal approval based on

    * Scientific content.

    * Researchers' competence.

    * Management Plan.

    * Periodic review.

- Independent investigators will have access to (nearly) all beamlines.

    * Fraction of reserved beamtime will depend on the nature of the collaborative team, negotiated at the time of proposal approval.

    * Access to this beamtime will be managed by the collaborative teams.

- Types of research permitted: open, proprietary, and classified.

TECHNICAL OBJECTIVES

- HIGH-BRILLIANCE SYNCHROTRON RADIATION FROM INSERTION DEVICES: 1-100 KEV

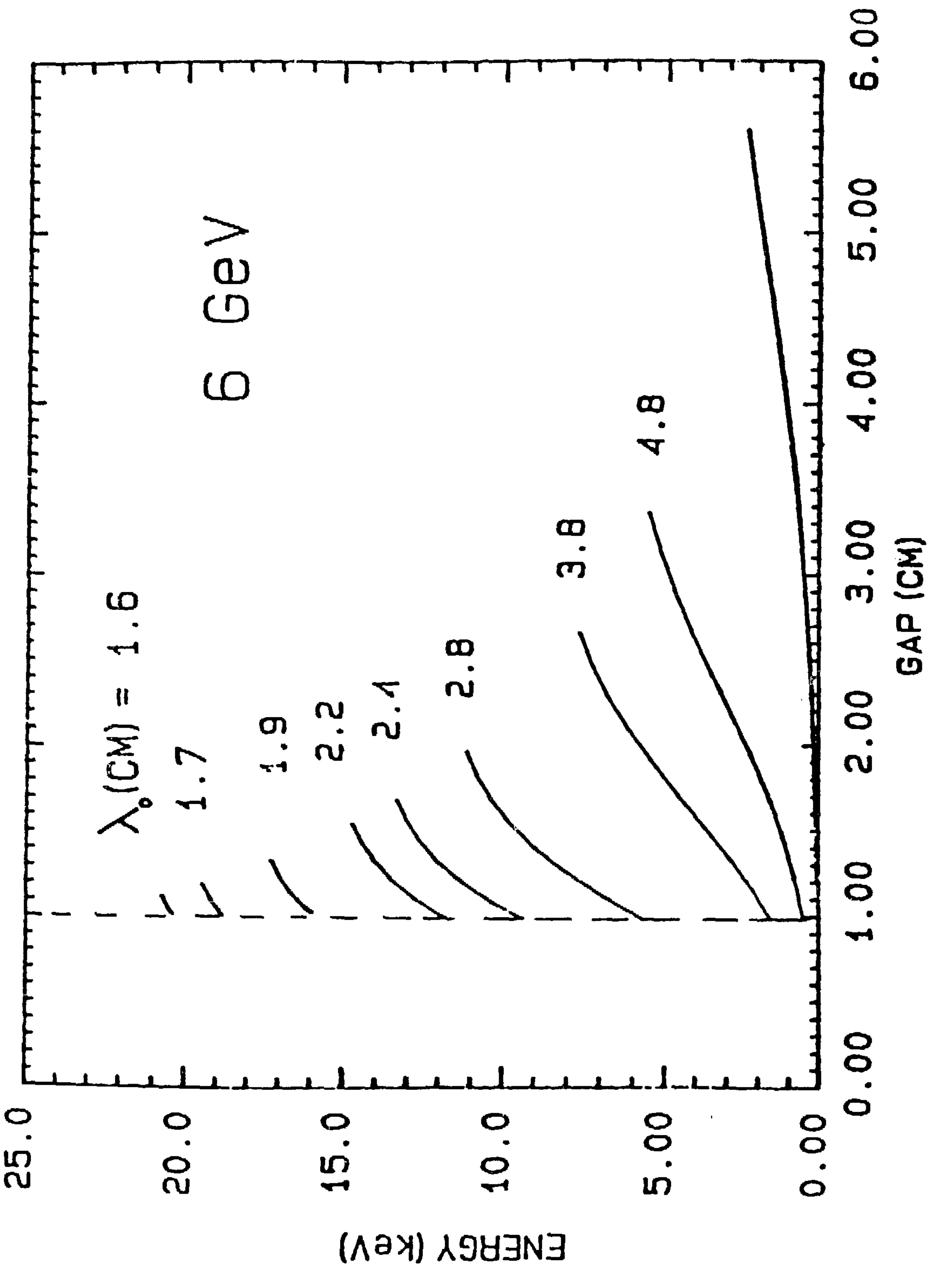
- HIGH STORED CURRENTS > 100 MAMPS

- LOW-EMITTANCE < 10NM-RAD

- FIRST UNDULATOR HARMONIC UP TO 20 KEV
  - ACCESS ALL ELEMENTS WITH K OR L EDGES
  - ENERGIES IMPORTANT FOR X-RAY DIFFRACTION

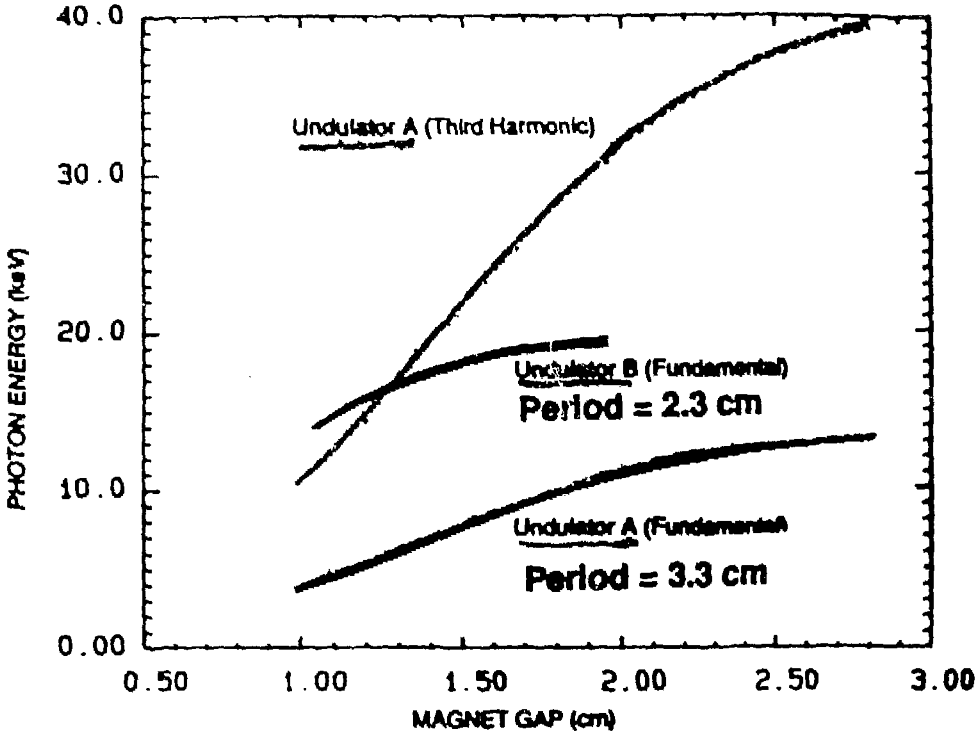
- UNDULATOR TUNABILITY WITH SINGLE DEVICE

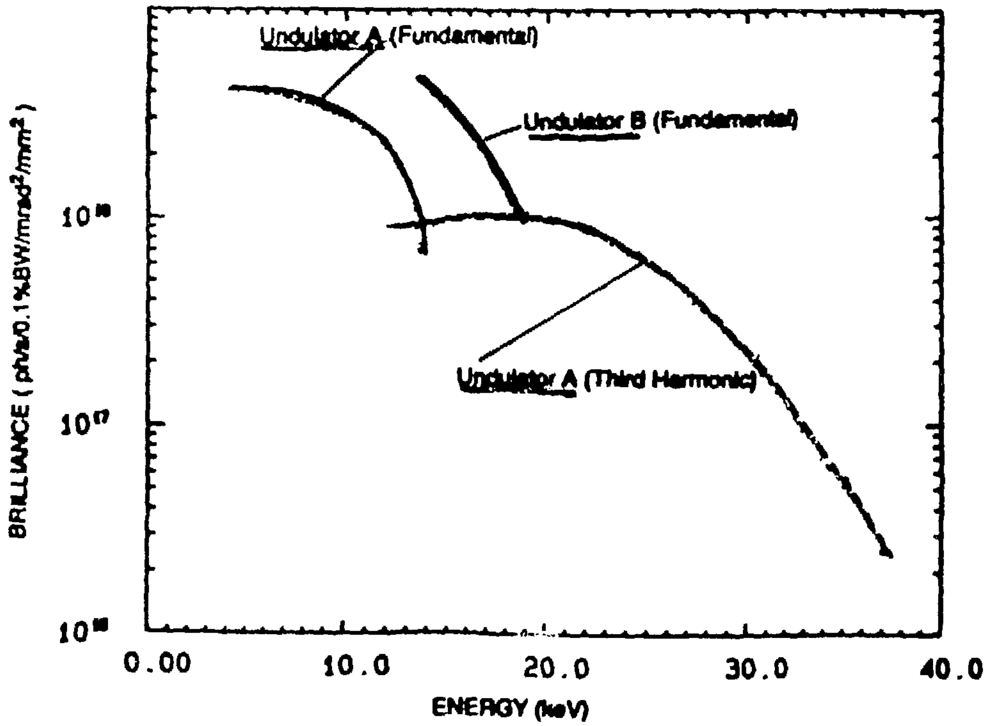
1ST HARMONIC	4.7 - 14 KEV
3RD HARMONIC	14 - 42 KEV

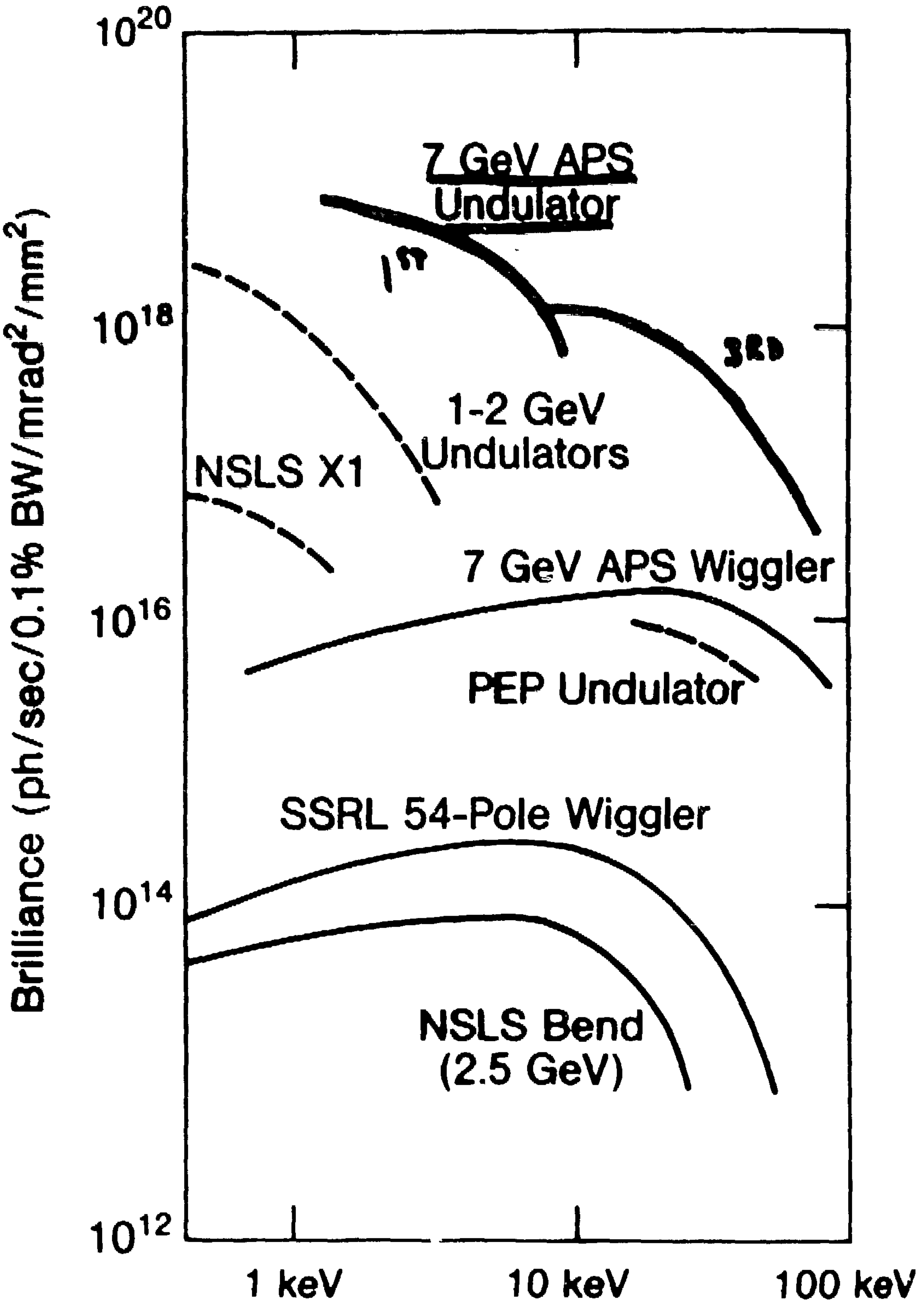


6 GeV
λ_0(CM) = 1.6
1.7
1.9
2.2
2.4
2.8
3.8
4.8
GAP (CM)
ENERGY (KeV)
0.00
1.00
2.00
3.00
4.00
5.00
6.00
0.00
5.00
10.0
15.0
20.0
25.0

Tunability of Undulators A and B



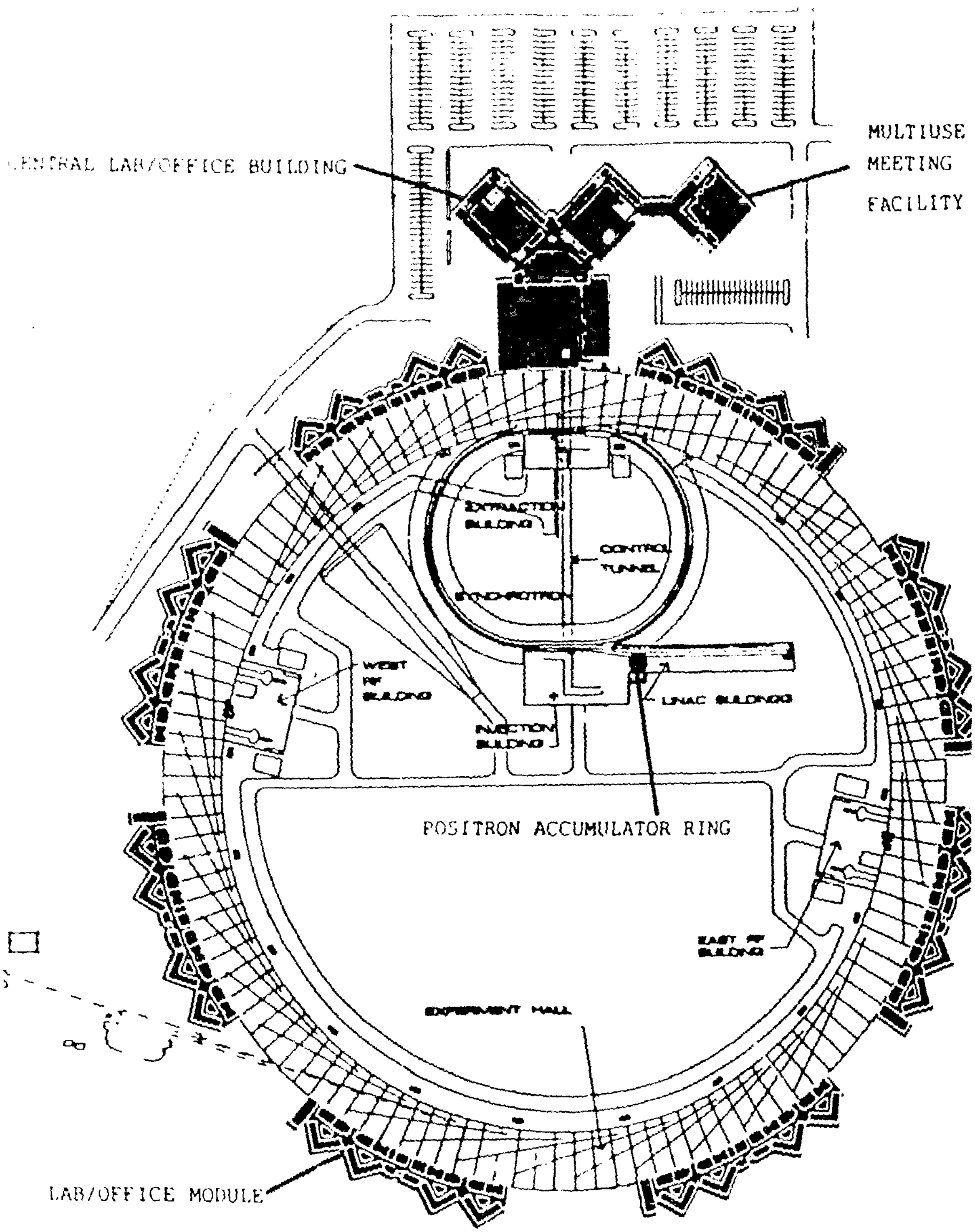




Brilliance (ph/sec/0.1% BW/mrad²/mm²)
10²⁰
10¹⁸
10¹⁶
10¹⁴
10¹²
7 GeV APS
Undulator
1ST
3RD
1-2 GeV
Undulators
NSLS X1
7 GeV APS Wiggler
PEP Undulator
SSRL 54-Pole Wiggler
NSLS Bend
(2.5 GeV)
1 keV
10 keV
100 keV

HIGHLIGHTS OF CHANGES

	6-GeV Design	7-GeV Design	% Change
Beamlines (#)	55	69	+26%
Construction Area (KSF)	596	679	+14%
Cost in FY86 M$ (including contingency)	304.52	309.25	+ 2%
Total Estimated Cost (including escalation)	375.94 ('88)	383.88 ('89)	+ 2%


CENTRAL LAB/OFFICE BUILDING
MULTIUSE MEETING FACILITY
EXTRACTION BUILDING
CONTROL TUNNEL
SYNCHROTRON
WEST RF BUILDING
INJECTION BUILDING
LINAC BUILDING
POSITRON ACCUMULATOR RING
EAST RF BUILDING
EXPERIMENT HALL
LAB/OFFICE MODULE

ACCELERATOR FACILITY

Linac	200 MeV e^- (3 amps) 450 MeV e^+ (15 mamps) Rep rate 60 Hz Length: 40 m
Accumulator	450 MeV DC ring Accumulate 24 linac pulses in 1/2 sec Damp positron emittance Circumference: 30 m
Booster	450 MeV $\rightarrow$ 7.7 GeV (1/3 sec) 1 sec rep rate Circumference: 367 m
Storage Ring	7.0 (0.7) GeV 100-300 mamps 40 periods 353 MHz 1248 buckets Lattice: Green-Chasman Circumference: 1060 m Filling time for 100mA less than min.

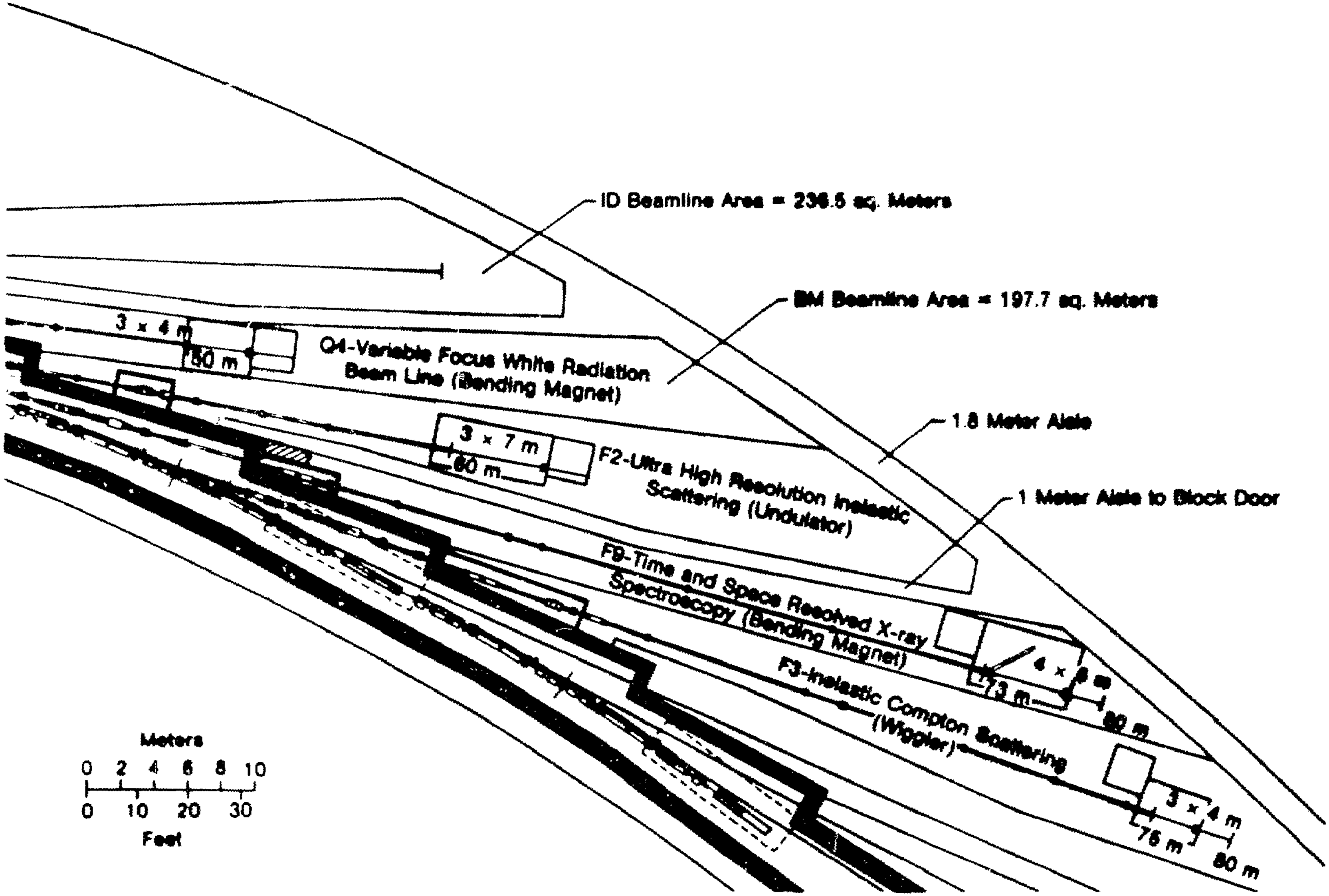
Experimental Facility:

Insertion Device Sources : 34

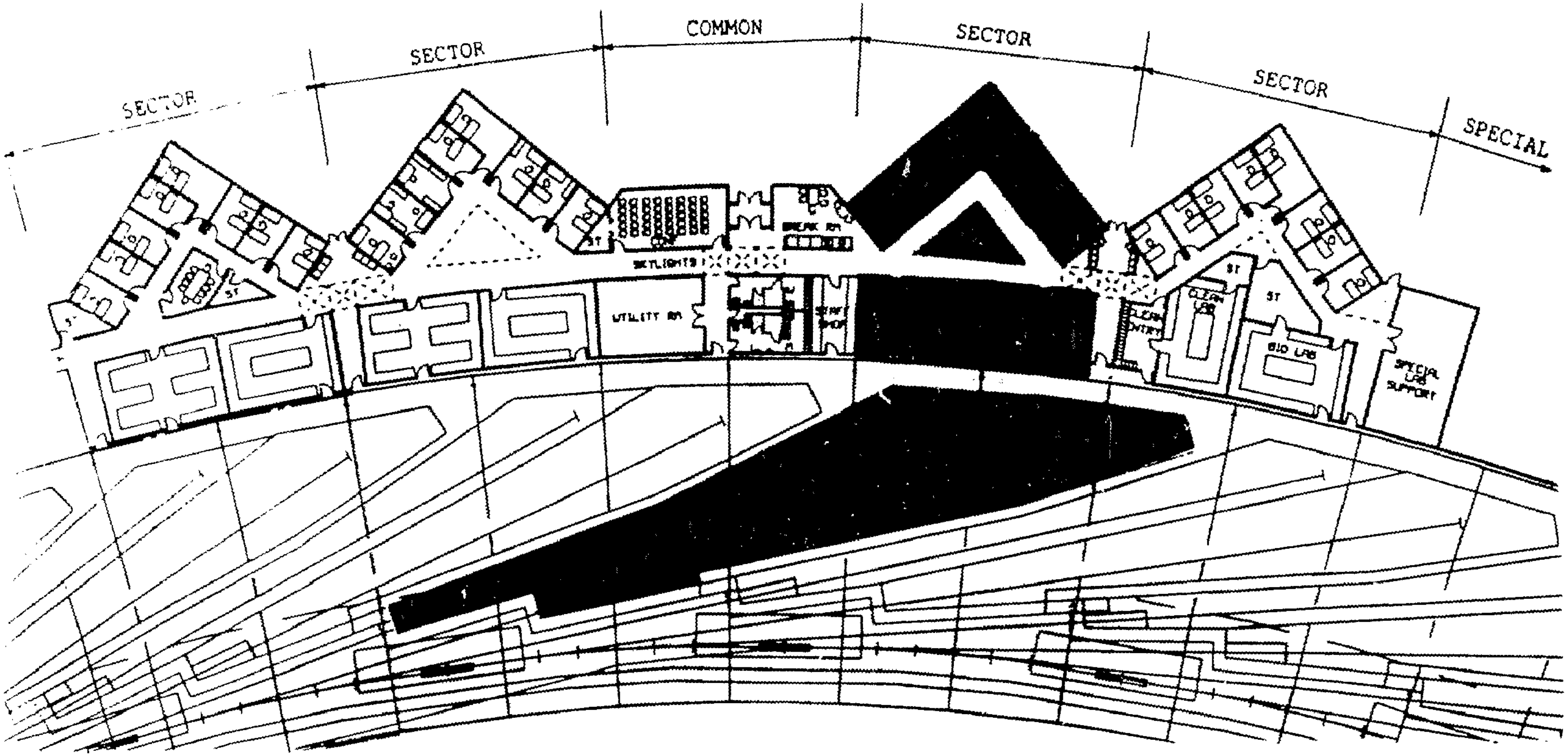
Bending Magnet Sources : 35

Total Sources : 69

Experimental Stations ~ 100


ID Beamline Area = 236.5 sq. Meters
BM Beamline Area = 197.7 sq. Meters
1.8 Meter Aisle
1 Meter Aisle to Block Door
3 x 4 m
80 m
Q4-Variable Focus White Radiation Beam Line (Bending Magnet)
3 x 7 m
80 m
F2-Ultra High Resolution Inelastic Scattering (Undulator)
F9-Time and Space Resolved X-ray Spectroscopy (Bending Magnet)
4 x 8 m
73 m
80 m
F3-Inelastic Compton Scattering (Wiggler)
3 x 4 m
75 m
80 m
Meters
0 2 4 6 8 10
0 10 20 30
Feet

User Lab / Office Module - 1988 Design



APS ACCELERATOR DESIGN*

Yanglai Cho
Argonne National Laboratory

Introduction

Project staff are seeking users' input to help guide our planning and tell us what is important for the commissioning and operation of the APS accelerator and experimental facilities. Progress has been made on the accelerator design since the first users meeting in terms of decisions on the storage-ring lattice and further refinements and improvements in prototyping activities, construction tolerances, and impedance budgets.

The present design calls for a 40-sector Chasman-Green type of lattice with a nominal operating energy of 7 GeV (7.5 GeV for initial operation). The hardware is to be capable of 7.7 GeV with a beam current of 280 mA. These specifications have been reviewed by the project's Accelerator Advisory Committee and by the DOE/ER Review Committee.

Current prototyping activities involve the vacuum system, the magnets, and the rf system. Lattice work continues, by means of computer modeling and calculations, with attention focused on construction tolerances. Impedance budgets are being improved to assure high-current operation.

Storage Ring, Injection, and Bunch Parameters

The main parameters specified at the Ames meeting have been modified to permit operation at 7 GeV. Since the present storage-ring design calls for 40 sectors instead of the 32 in the Ames parameters, there are also 40 straight sections, of course. Of these straight sections, three will be used for rf cavities, one for injection, and one for beam-abort and other accelerator physics applications, leaving 35 available for insertion-device (ID) beam lines in the experimental area layout. The lattice element-to-element length is 6.2 m, while the straight-section length available for IDs is 5.2 m. For longer devices, a length of 8 m can be achieved by removing one quadrupole magnet from each end.

In 1987, the DOE/ER Review Committee recommended that we study a possible shortening of the filling time for injection of positrons into the booster synchrotron; the committee added $4 million to the project's cost to support this change. In the 1987 APS Conceptual Design Report (CDR-87), the

*The summary presented here is based on notes taken at the meeting.

booster had a "cold" filling time of 4 min, with an overall efficiency of about 40%. In our new filling scheme, a 30-m-circumference positron accumulator ring (PAR) between the linac and the booster shortens this time by a factor of six.

With respect to bunch separation and bunch current, the present design goal is 5 mA per bunch or greater. At 5 mA per bunch, 20 bunches would mean 100-mA operation (60 bunches, 300 mA). (The number of rf buckets available in the ring is 1248.) Bunch separation in the 20-bunch mode would be 177 ns. These bunch separations and currents are intended for "timing" experiments.

Vacuum Chamber System

Our first priority in prototyping activities has been to assure the constructibility and serviceability of the vacuum system. Studies of chamber surface cleaning using the LEP method are under way. We plan to use both active and passive systems to prevent overheating by mis-steering of the photon beam. The active system monitors machine conditions and dumps the stored beam if mis-steering exceeds some specified limit.

The passive protection system, which is more interesting, is based on a built-in orbit-correction scheme. This scheme involves using highly accurate feedback on the photon beam (both position and angle) to determine adjustments to correction-magnet field strengths and positions that will correct the orbit of the circulating beam. (Photon-beam-position feedback accuracy depends on the accuracy of photon detection; we need help from users on this.) Magnets available include eight horizontal correction magnets, plus two in the dipoles, and nine vertical correction magnets; we can use four plus four for orbit correction and another four plus four for ID beam feedback. The design goals are to limit (vertical) corrector strengths to less than 0.25 mrad, so that the photon beam cannot strike the chamber wall, and to provide vertically adjustable quadrupole mounts.

Commissioning and Operating Considerations

It is not too early to consider plans for commissioning and operating the APS accelerator systems, and we request user input to these plans. Retrofitting is both expensive and painful, so we prefer to do our planning now. That is one of the principal reasons for our building a full-scale mock-up of one sector of the storage ring; this mock-up, which you will see later today in the Building 362 High Bay, shows us what to avoid as we refine the design.

On the basis of past experience with accelerator facilities, we are planning not to run the APS at the hardware limits; thus, we have a built-in reserve. We are also planning, particularly for the commissioning period, to have adequate, even redundant, diagnostic equipment.

With respect to hardware, the straight-section vacuum chamber segments (designed to have much narrower apertures than segments in the bending-magnet sections) will be built in three different sizes: normal ring-chamber aperture, for Day 1 operation; 1.4-cm aperture, for early operation; and 1.0-cm aperture, for operation during system maturity. Since initial operation will be with electrons rather than positrons in the circulating beam, all magnet power supplies will have reversible switches for electron operation.

Except for the first day, we plan no lock-out of the experimental area during routine operation. Instead, sufficient lead shielding will be provided for local shielding if needed.

Start-Up Considerations

At start-up, while we search for the optimal operating point and make corrections to the beam orbit, we will be able to detune the lattice to facilitate orbit corrections. The machine will be operated at low intensity for beam diagnostics. If photon beam scrubbing of the chamber is needed, we may use an electron beam for this purpose.

As was noted above, at start-up the straight sections will contain vacuum-chamber segments of large (normal) aperture. At the time of ID installation, we plan to install chambers with 1.4-cm aperture at some reasonable current (say, 50 mA) using sector valves; at this point, during the initial experiments, the ring would be run at 7.5 GeV. Later, when the "golden orbit" is achieved, the smaller, 1.0-cm-aperture chambers will be installed.

ENERGY AND TIME STRUCTURE OF PHOTONS FROM APS INSERTION DEVICES*

Gopal K. Shenoy
Argonne National Laboratory

Today I would like to point out some of the highlights of the current designs with respect to insertion devices and beam lines and bring you up to date on the R&D activities we are planning. The ultimate goals, as you know, are spatial brightness and spectral brightness. We are looking for (1) a large number of x-rays in a very small solid angle and (2) large density with extremely narrow bandwidth, and this is accomplished using undulators.

Within a given undulator, the change in the energy of the photons produced is a function of the deflection parameter K, which is proportional to the magnetic field and the period. The period gets Lorentz-transformed twice to get to the range from a few centimeters to a few Angstroms; it is proportional to E squared. As for the magnetic field, you open up the jaws of the undulator to increase the gap and decrease the field. When you decrease the magnetic field, K decreases and so does the photon energy. Now, we have plotted minimum magnet gap as a function of ring energy, and the resulting curve, which represents first-harmonic tunability from 4.7 to 14 keV, tells us we need to operate the ring at 7 GeV and with a 1-cm gap to achieve that tunability.

For a complete Monte Carlo calculation of spectral brilliance, as you change the gap of this undulator (period of 3.3 cm, K = 2.2), K changes and the first-harmonic peak moves along an envelope. Later on, the third harmonic starts to appear, so you can cover the range farther on using the third harmonic. We have plotted brilliance as a function of energy for that undulator, which we call Undulator A; with it, we lose roughly two orders of magnitude in going from 4 to 40 keV. This is the sort of device that can be utilized by most people, and if we produce a lot of them we can do so economically. If this range can meet the needs of most of the synchrotron community, then I think it is the one to go with.

A 2.3-cm-period undulator, called Undulator B, will produce higher brilliance at higher photon energy and may be useful for some experiments. Now, a certain number of experiments are brilliance-intensive, while others are flux-intensive. For people who are more interested in flux than in brilliance, I have a curve that shows flux through a pinhole. You can get 10^{14}-10^{15} photons per second through the pinhole. The angular divergence is on the order of 9 microradians vertically and 24-25 microradians horizontally. To translate this, that's a spot less than a millimeter in size 50 meters from the source point.

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*The summary presented here is based on notes taken at the meeting; viewgraphs were provided by the speaker.

Let me consider wiggler sources. Almost all wiggler sources on this 7-GeV ring can be built using permanent magnet technology. You can get critical energies up to 60 kilovolts with permanent magnet technology, so you can get radiation at a few hundred keV and a fair amount of flux and brilliance without any trouble.

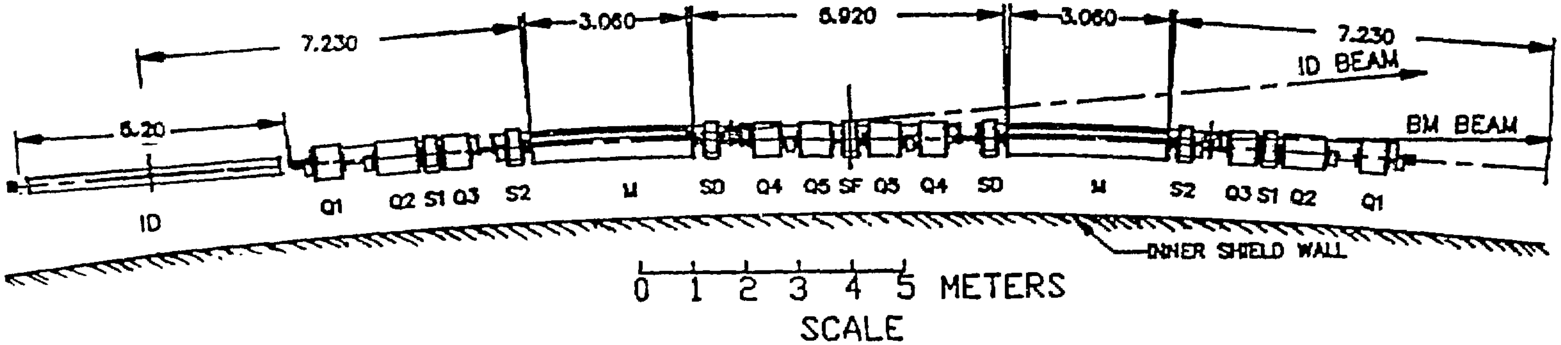
Here are two designs. One has a 33-kilovolt critical energy; this, of course, corresponds to the hard-ion edge, in which biologists are taking a lot of interest. The other is a 10-kilovolt critical-energy wiggler; this is not your typical wiggler, because here we're reducing the critical energy of the radiation coming out and making it less than that produced by bending magnets (19 kilovolts). In addition, the angular opening of this wiggler's radiation is considerably smaller than what we are used to at current facilities.

We have been thinking about special devices of interest for specific kinds of experiments. One functions as an undulator in the low-energy range, about 2-7 keV, and then as you close the gap it becomes a 10-keV critical-energy wiggler. You can also build a wiggler with vertical polarization; this is fairly straightforward to build around the proposed APS insertion-device vacuum chambers. We are also looking into a wiggler for producing elliptical radiation.

We had a workshop here recently that raised the issue of time structure, and we're addressing some questions on that. A single-bunch mode is ideal for some experiments (there is a whole class of experiments related to this, depending on the excitation process), but most users are interested in the multibunch mode, simply because it produces more flux. We are considering loading the storage ring with say, a lone bunch on one side and 19 bunches on the other side and having a chopper synchronized with the single bunch. With a 5-mA current in this bunch and the rest in the remaining bunches, the typical user won't see much difference between this mode and normal operation, while the single-bunch experimenter can use a chopper outside the beam line to get dark times (when you don't see an x-ray) for several microseconds.

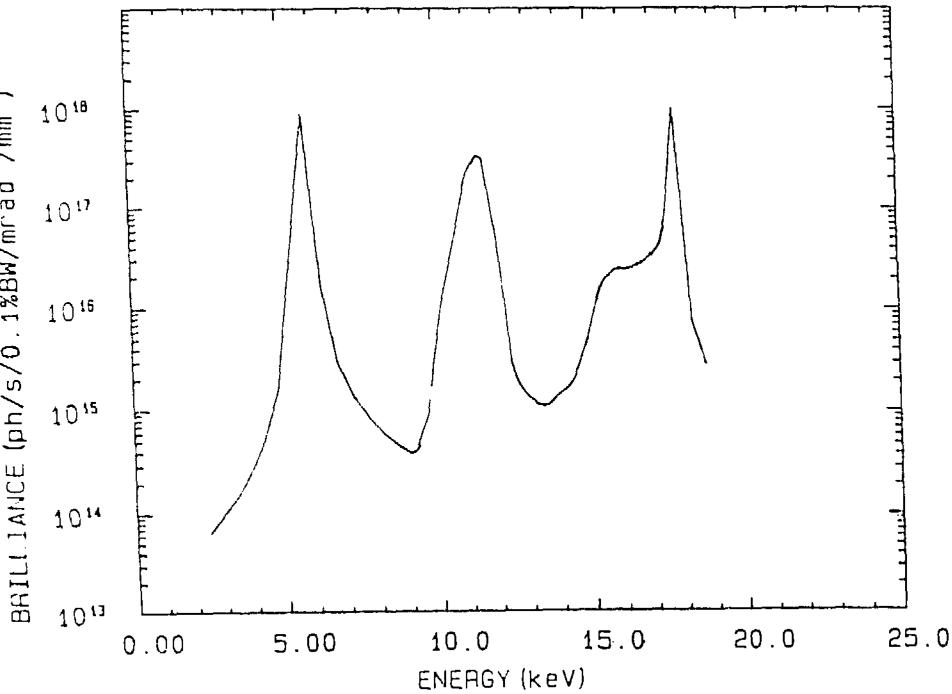
On the 3.3-cm insertion device, we have developed a prototype in collaboration with Cornell. This device, which is 2 meters long, is now being built and will be tested on CESR in a month or so using a special low-emittance mode (actually eight or nine times larger than the anticipated APS emittance). And so we will have some firsthand experience at getting this radiation and testing it out.

Another issue is power. When a large heat load hits an optical surface, there are distortions of the surface and distortions from the rocking curve. Of course, you will be taking this radiation at an appropriate Bragg angle, but this is still not enough to relieve the heat problem. We have developed a liquid gallium electromagnetic induction pump -- there are no moving parts in it -- and it is functioning. Two weeks ago this pump was taken to Cornell, and a very useful experiment was carried out. Bob Smither is leading this effort.

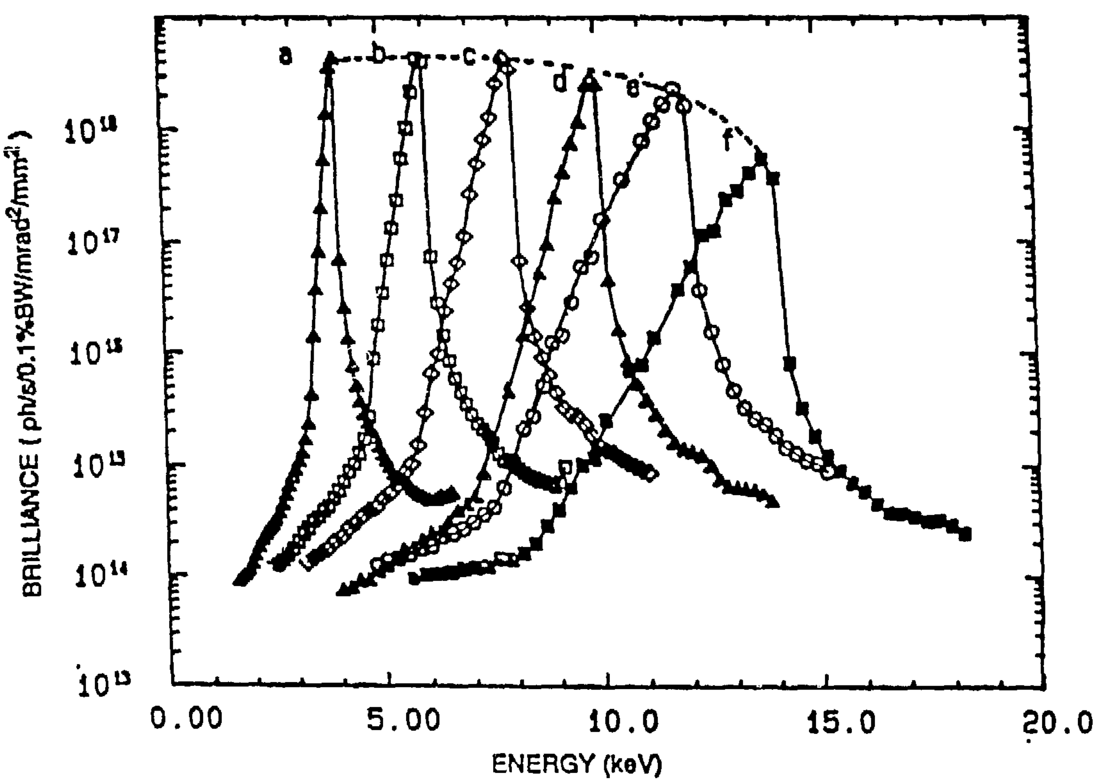


Location of Insertion-Device and Bending-Magnet Sources

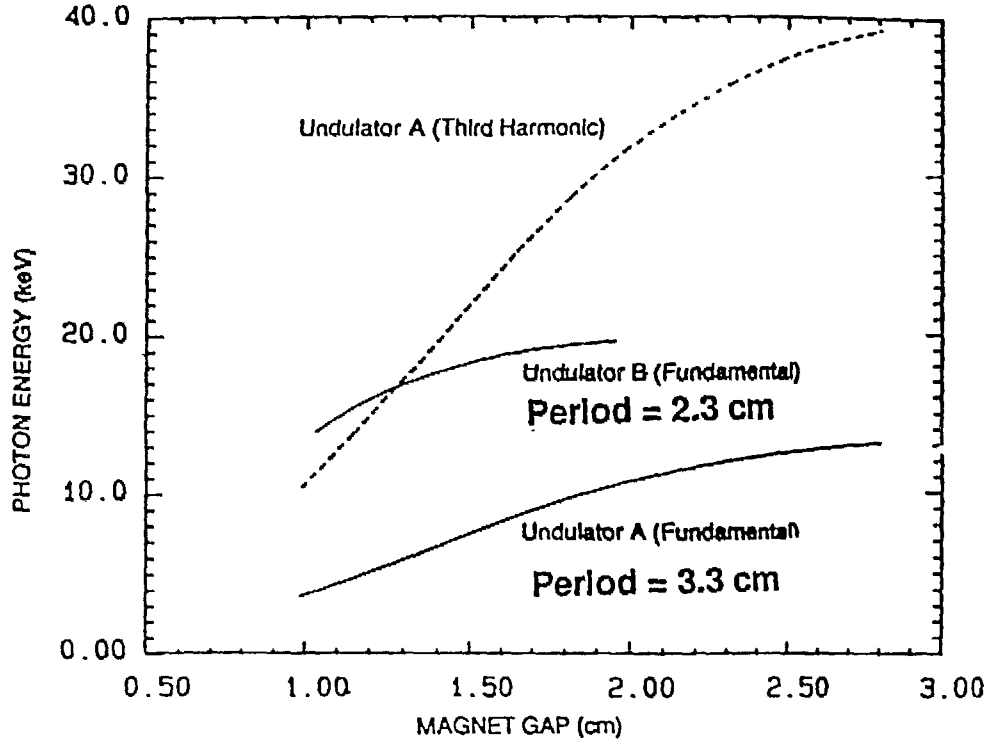
TYPICAL SPECTRUM FROM UNDULATOR A (PERIOD = 3.3 cm)
GAP = 1.3 cm, K = 1.65

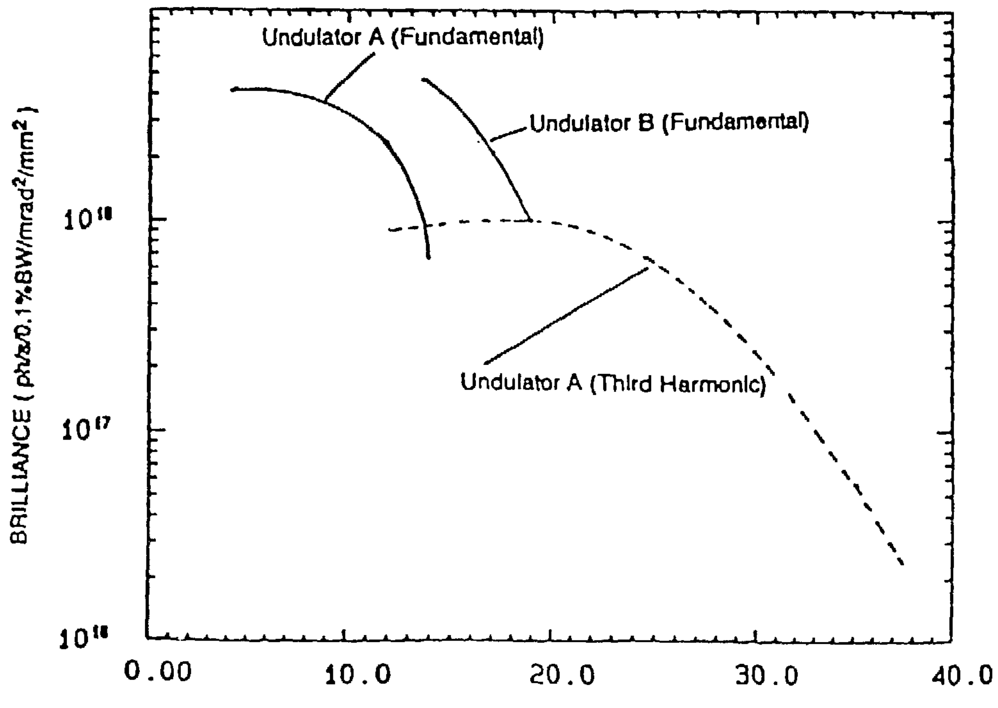


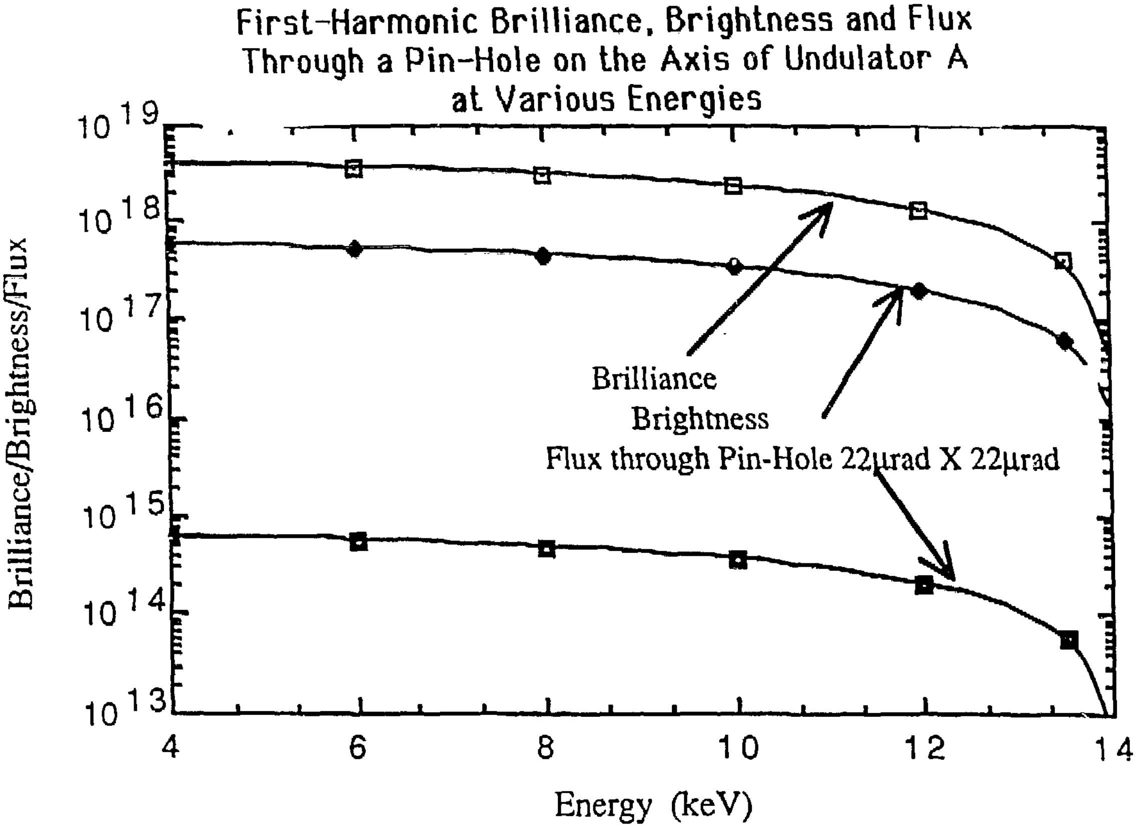
Tunability of Undulator A (Period - 3.3 cm)

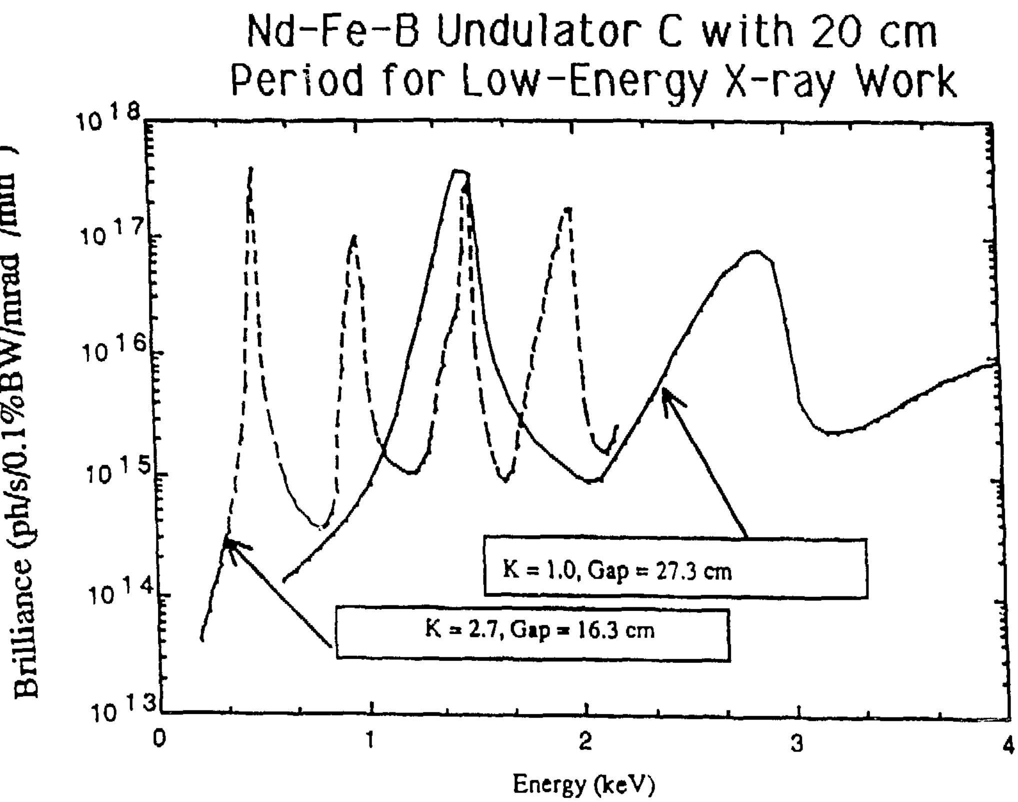


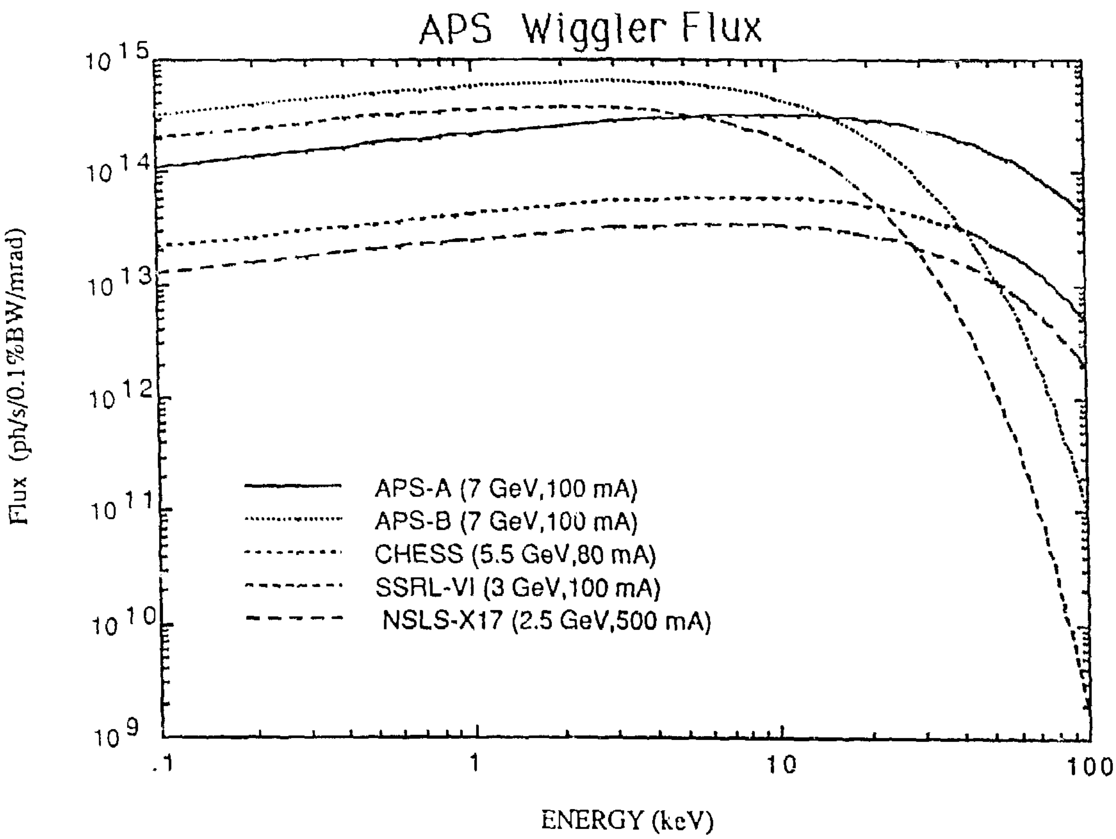
Tunability of Undulators A and B

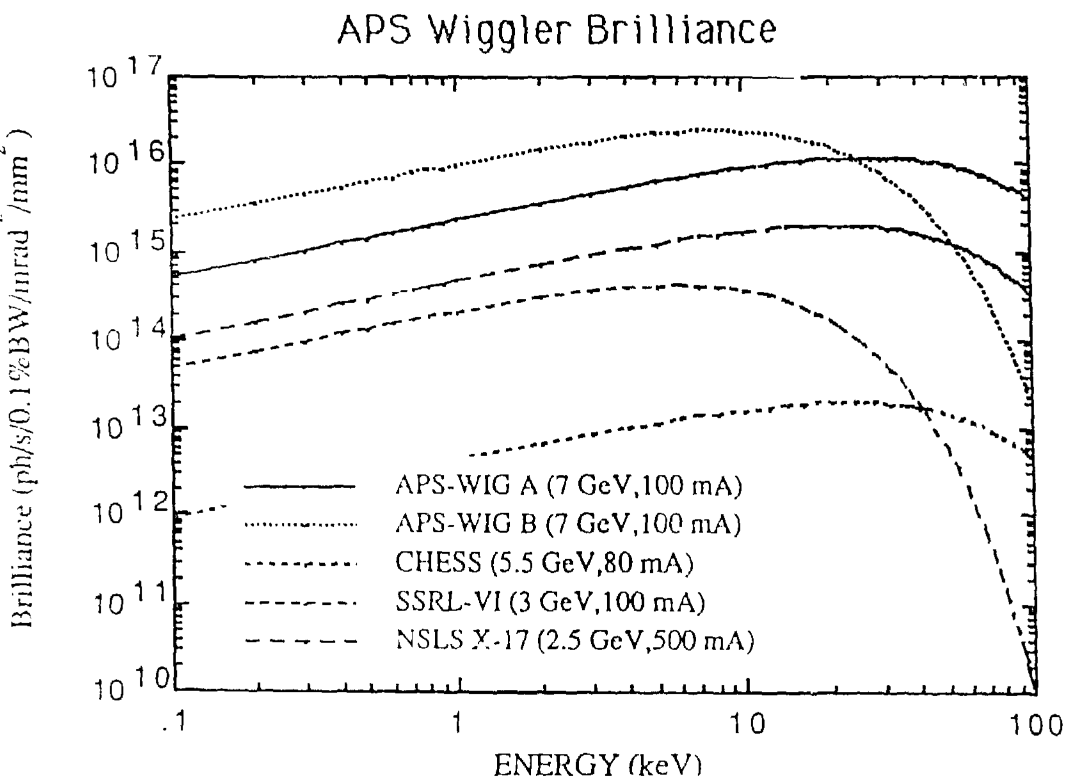


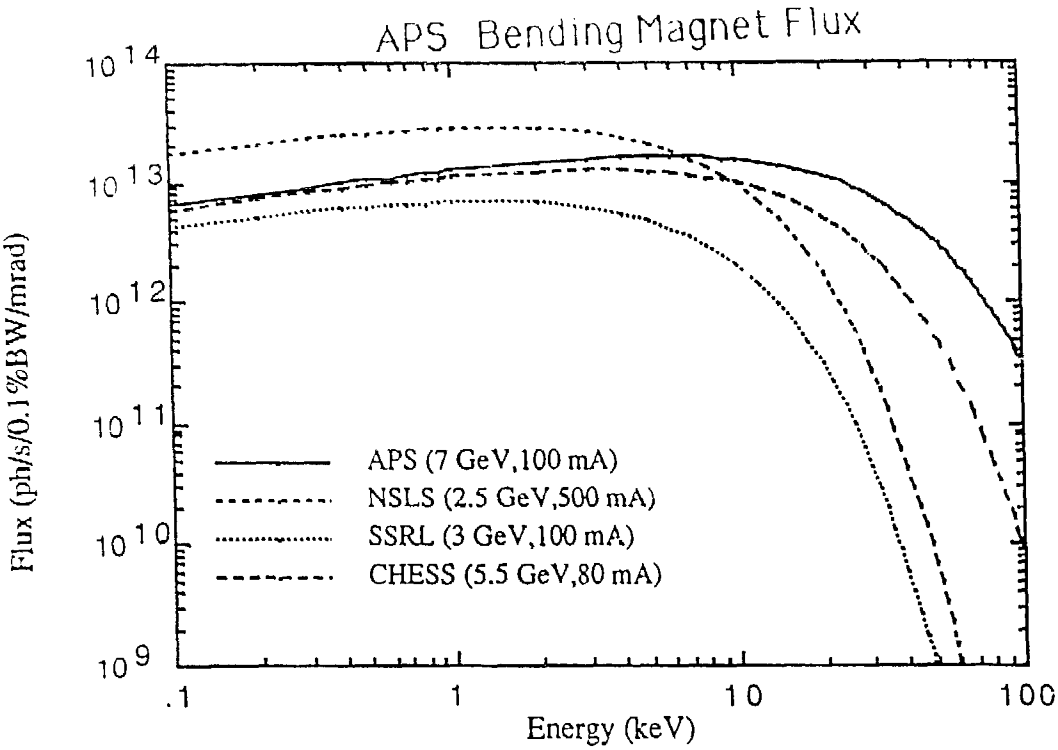


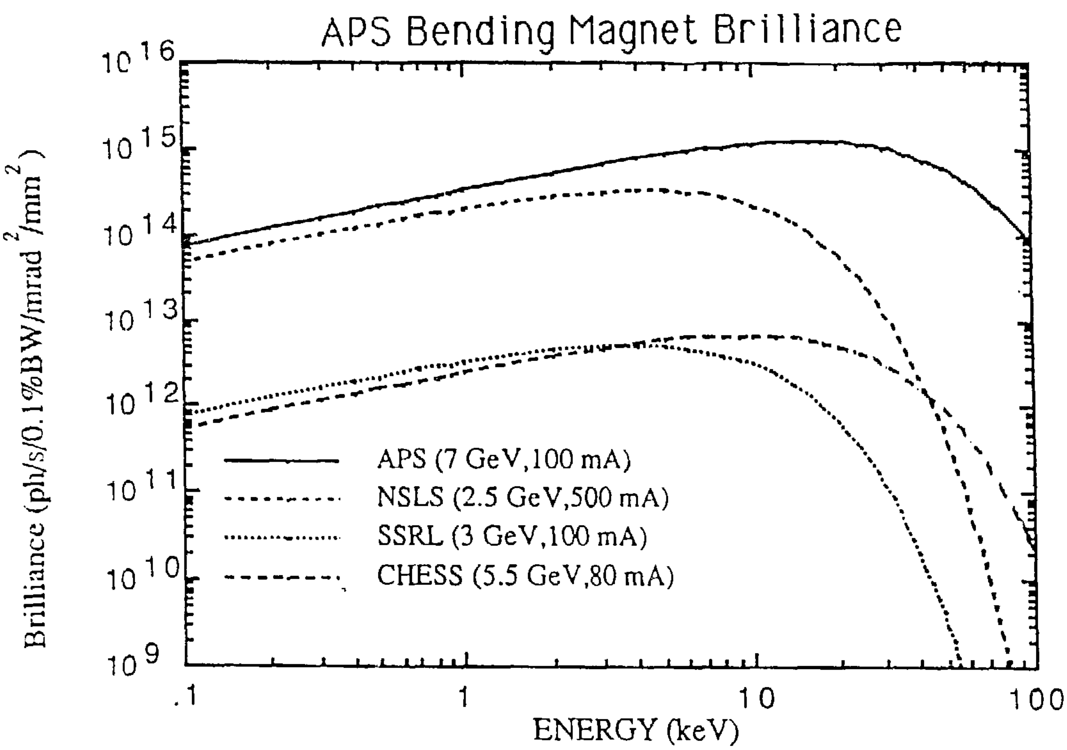

First-Harmonic Brilliance, Brightness and Flux
Through a Pin-Hole on the Axis of Undulator A
at Various Energies
Brilliance/Brightness/Flux
Brilliance
Brightness
Flux through Pin-Hole 22μrad X 22μrad
Energy (keV)

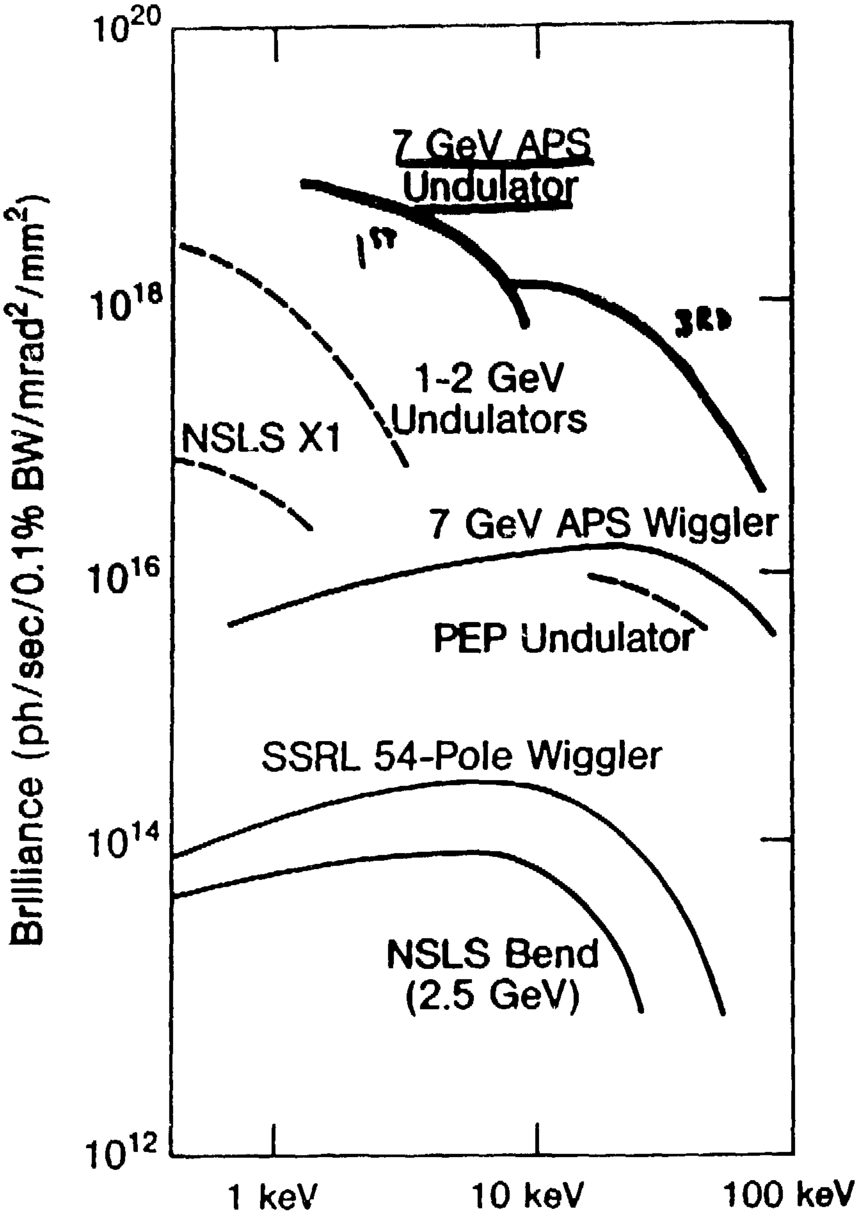

Nd-Fe-B Undulator C with 20 cm
Period for Low-Energy X-ray Work
Brilliance (ph/s/0.1%BW/mrad²/mm²)
K = 1.0, Gap = 27.3 cm
K = 2.7, Gap = 16.3 cm
Energy (keV)


APS Wiggler Flux
Flux (ph/s/0.1%BW/mrad)
10 15
10 14
10 13
10 12
10 11
10 10
10 9
.1
1
10
100
ENERGY (keV)
APS-A (7 GeV,100 mA)
APS-B (7 GeV,100 mA)
CHESS (5.5 GeV,80 mA)
SSRL-VI (3 GeV,100 mA)
NSLS-X17 (2.5 GeV,500 mA)

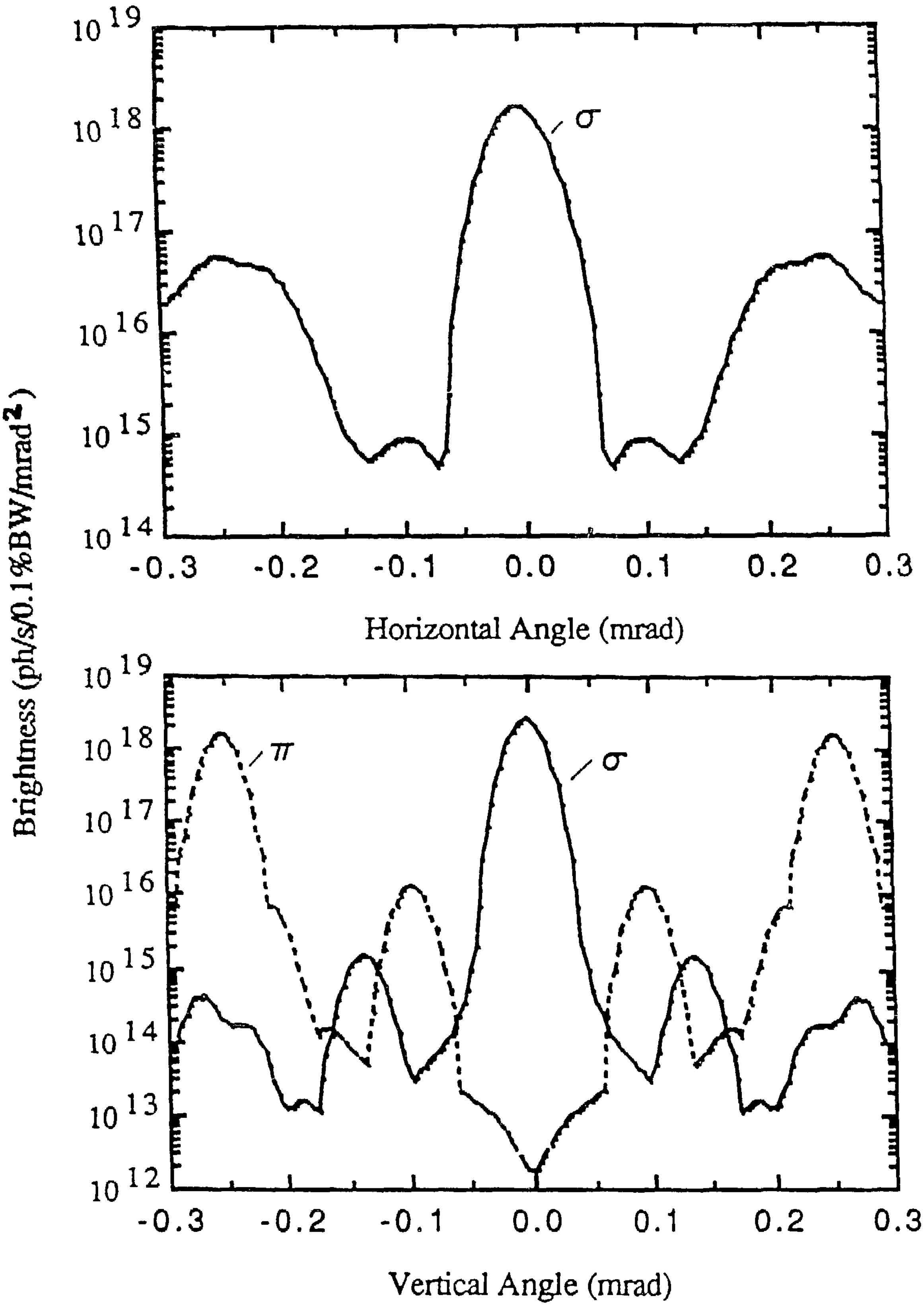

APS Wiggler Brilliance
Brilliance (ph/s/0.1%BW/mrad 2 /mm 2)
10 17
10 16
10 15
10 14
10 13
10 12
10 11
10 10
.1
1
10
100
ENERGY (keV)
APS-WIG A (7 GeV,100 mA)
APS-WIG B (7 GeV,100 mA)
CHESS (5.5 GeV,80 mA)
SSRL-VI (3 GeV,100 mA)
NSLS X-17 (2.5 GeV,500 mA)

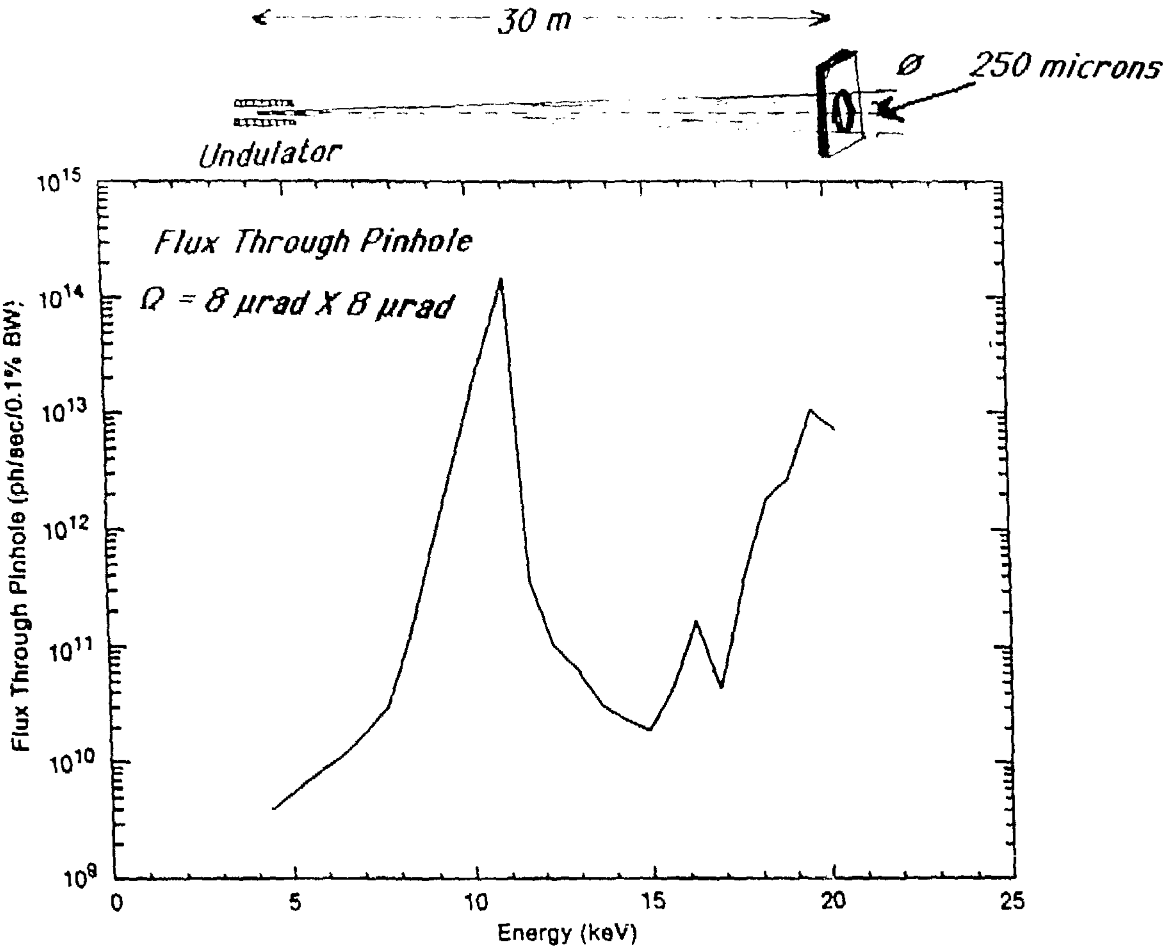

APS Bending Magnet Flux
Flux (ph/s/0.1%BW/mrad)
10 14
10 13
10 12
10 11
10 10
10 9
.1
1
10
100
Energy (keV)
APS (7 GeV,100 mA)
NSLS (2.5 GeV,500 mA)
SSRL (3 GeV,100 mA)
CHESS (5.5 GeV,80 mA)

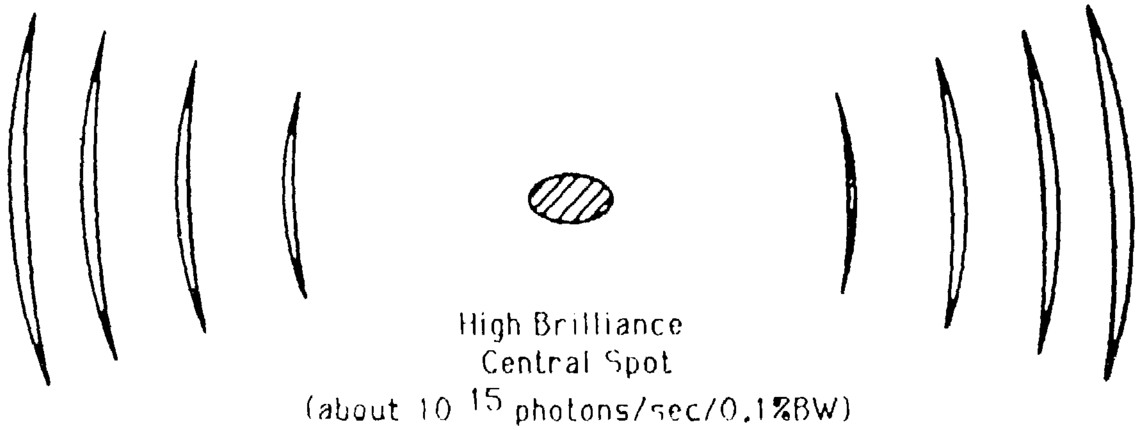

APS Bending Magnet Brilliance
Brilliance (ph/s/0.1%BW/mrad²/mm²)
10 16
10 15
10 14
10 13
10 12
10 11
10 10
10 9
.1
1
10
100
ENERGY (keV)
APS (7 GeV,100 mA)
NSLS (2.5 GeV,500 mA)
SSRL (3 GeV,100 mA)
CHESS (5.5 GeV,80 mA)



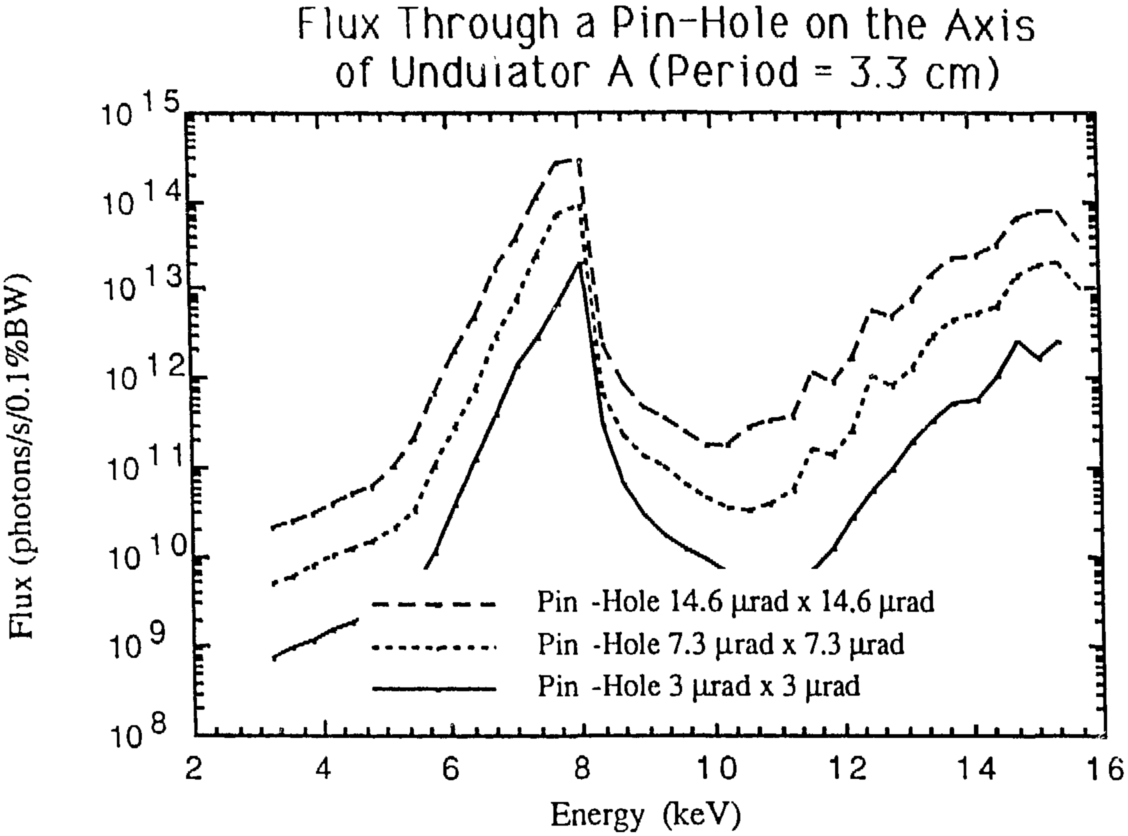
Brilliance (ph/sec/0.1% BW/mrad²/mm²)
10²⁰
10¹⁸
10¹⁶
10¹⁴
10¹²
1 keV
10 keV
100 keV
7 GeV APS
Undulator
1ST
3RD
1-2 GeV
Undulators
NSLS X1
7 GeV APS Wiggler
PEP Undulator
SSRL 54-Pole Wiggler
NSLS Bend
(2.5 GeV)


Brightness (ph/s/0.1%BW/mrad²)
10 19
10 18
10 17
10 16
10 15
10 14
σ
-0.3
-0.2
-0.1
0.0
0.1
0.2
0.3
Horizontal Angle (mrad)
10 19
10 18
10 17
10 16
10 15
10 14
10 13
10 12
π
σ
-0.3
-0.2
-0.1
0.0
0.1
0.2
0.3
Vertical Angle (mrad)



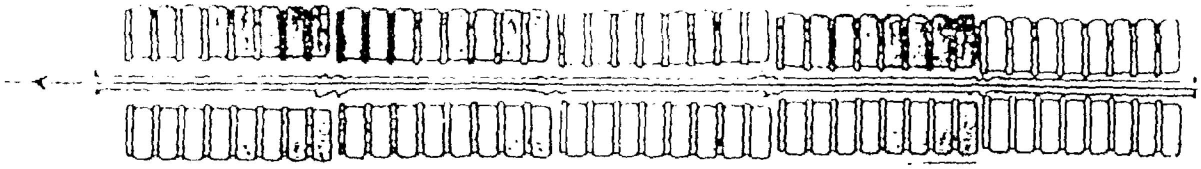


Source Size:
85 μm X 308 μm
9 μrad X 24 μrad



Flux Through a Pin-Hole on the Axis
of Undulator A (Period = 3.3 cm)
10 15
10 14
10 13
10 12
10 11
10 10
10 9
10 8
Flux (photons/s/0.1%BW)
2
4
6
8
10
12
14
16
Energy (keV)
Pin -Hole 14.6 µrad x 14.6 µrad
Pin -Hole 7.3 µrad x 7.3 µrad
Pin -Hole 3 µrad x 3 µrad

BROAD BAND UNDULATOR

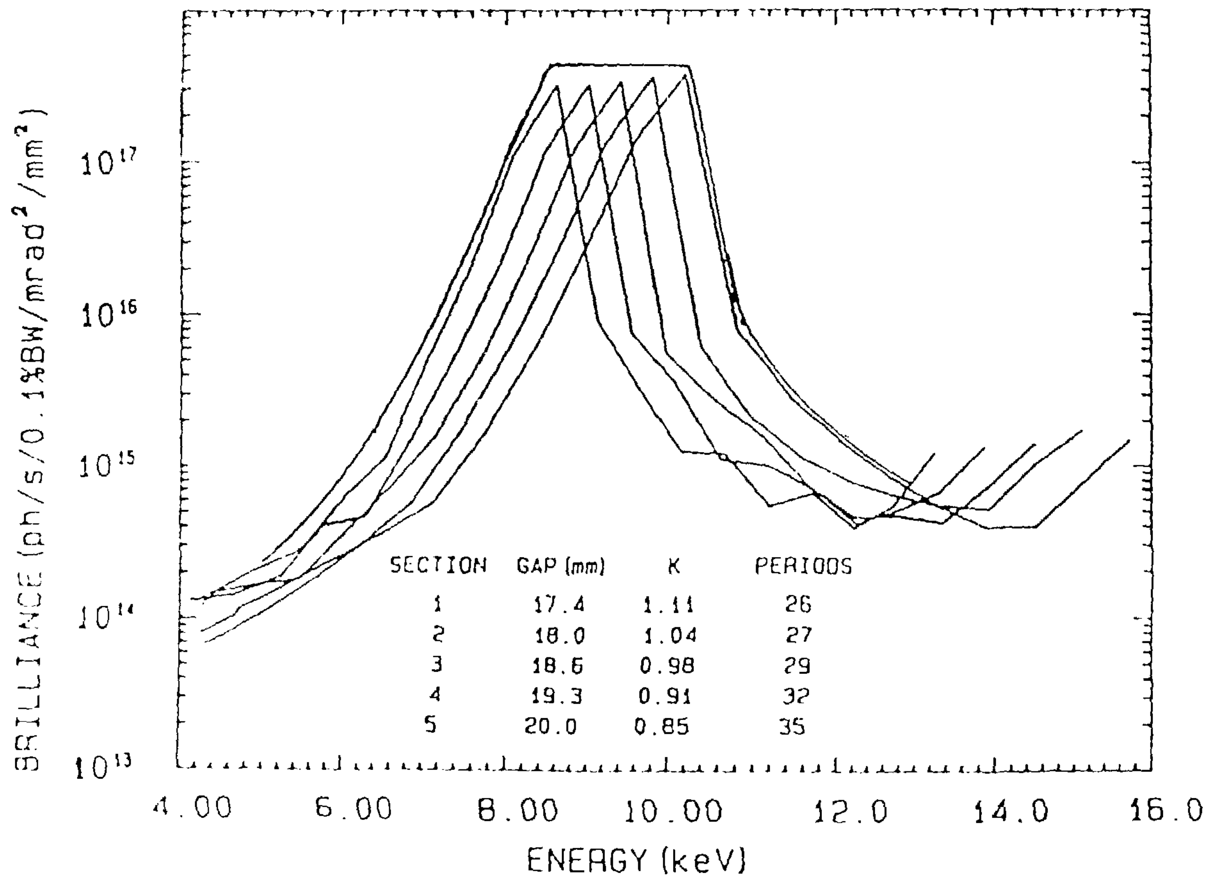


GAP (mm)	20.0	19.3	18.6	18.0	17.4
PERIOD	35	32	29	27	26

FLAT-TOP ENERGY RANGE = 1 keV

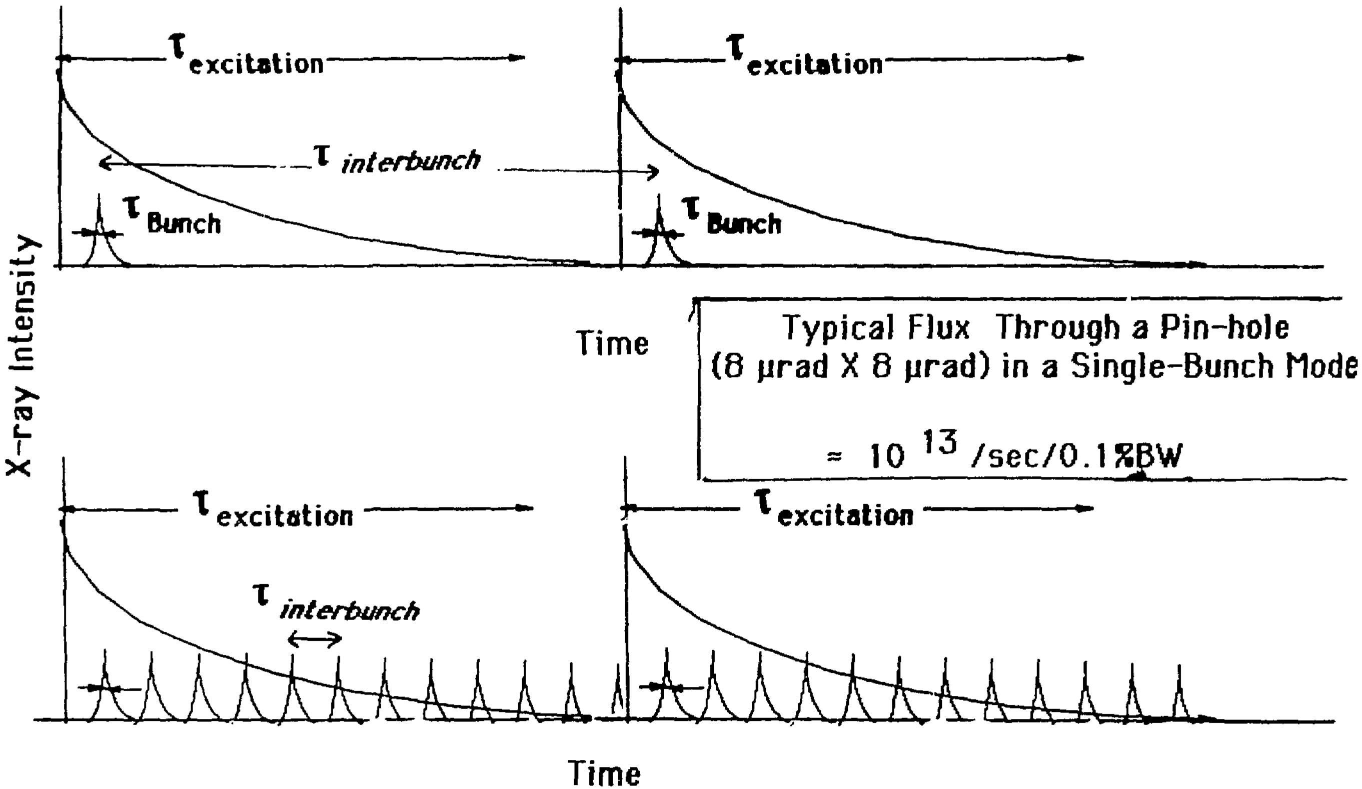
BROAD-BAND UNDULATOR

7.0 GeV 100 mA Period = 3.35 cm



Time Structure of the Advanced Photon Source

Bunch Length	116 ps (2xrms)
Orbital Period	3526 ns
Interbunch Period	
1 Bunch	3536 ns (max 5 mA)
20 Bunches	177 ns (100 mA total)
60 Bunches	59 ns (100 mA total)

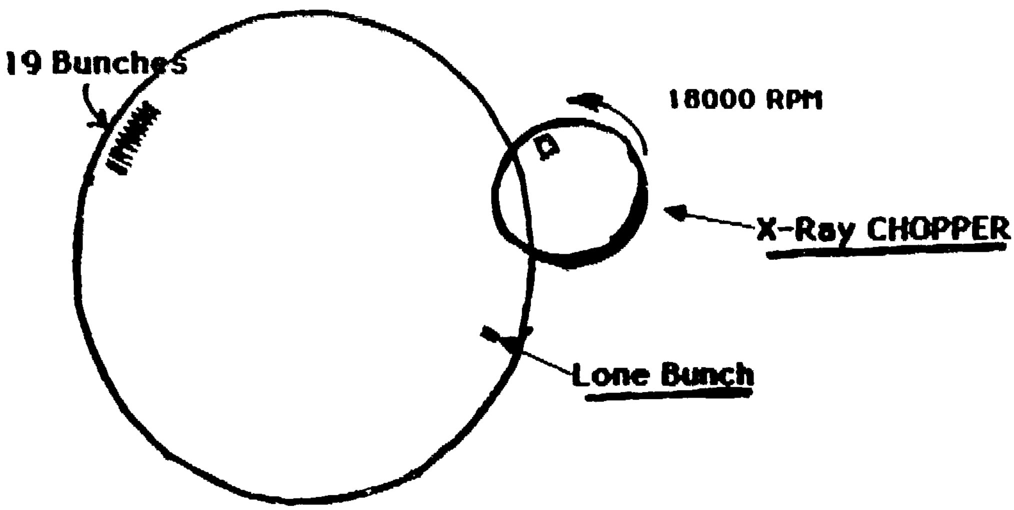

τ excitation
τ interbunch
τ Bunch
τ excitation
τ Bunch
X-ray Intensity
Time
Typical Flux Through a Pin-hole
(8 μrad X 8 μrad) in a Single-Bunch Mode
≈ 10 13 /sec/0.1%BW
τ excitation
τ excitation
τ interbunch
Time

Flux per Bunch for APS X-ray Sources

Source	Energy (keV)	Flux X-rays/bunch/0.1% BW
BM	19	1.7×10^6 /mrad θ
Wiggler A	33	3.9×10^7/mrad θ
Wiggler B	10	4.5×10^7/mrad θ
Undulator A	8	2.1×10^8
Undulator B	14	1.7×10^8

Use of X-ray Chopper

Storage Ring / Asymmetrically Spaced Bunches



Total Bunches		20
Maximum Current		100 mA
Current in the Lone Bunch		5 mA
Lone Bunch Duration		116 ps
Dark Time Using X-ray		
Chopper:	Min	3.56 µsec
	Max	3.33 msec
(for 18000 RPM)		

PRE-MONOCHROMATOR R&D

Cooling with Liquid Gallium
Bob Smither: Argonne

A. Design, Construction and Testing of Liquid Ga Pumps:

   Bob Smither: Argonne
   George Forster: Argonne

B. Optimization of Crystal Geometries with Finite-element Analysis

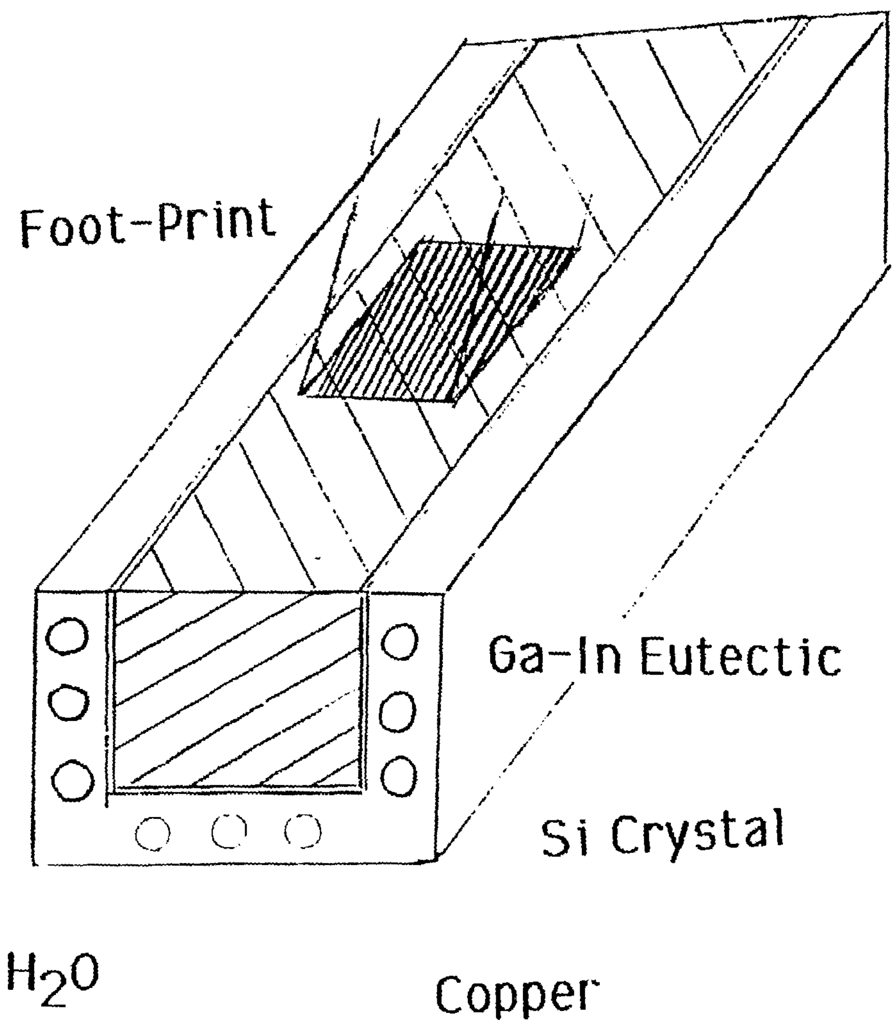
   Ali Khounsari
   Christian Kot
   Tuncer Kuzay
   Denny Mills
   Bob Smither
   Jim Viccaro
   } Argonne

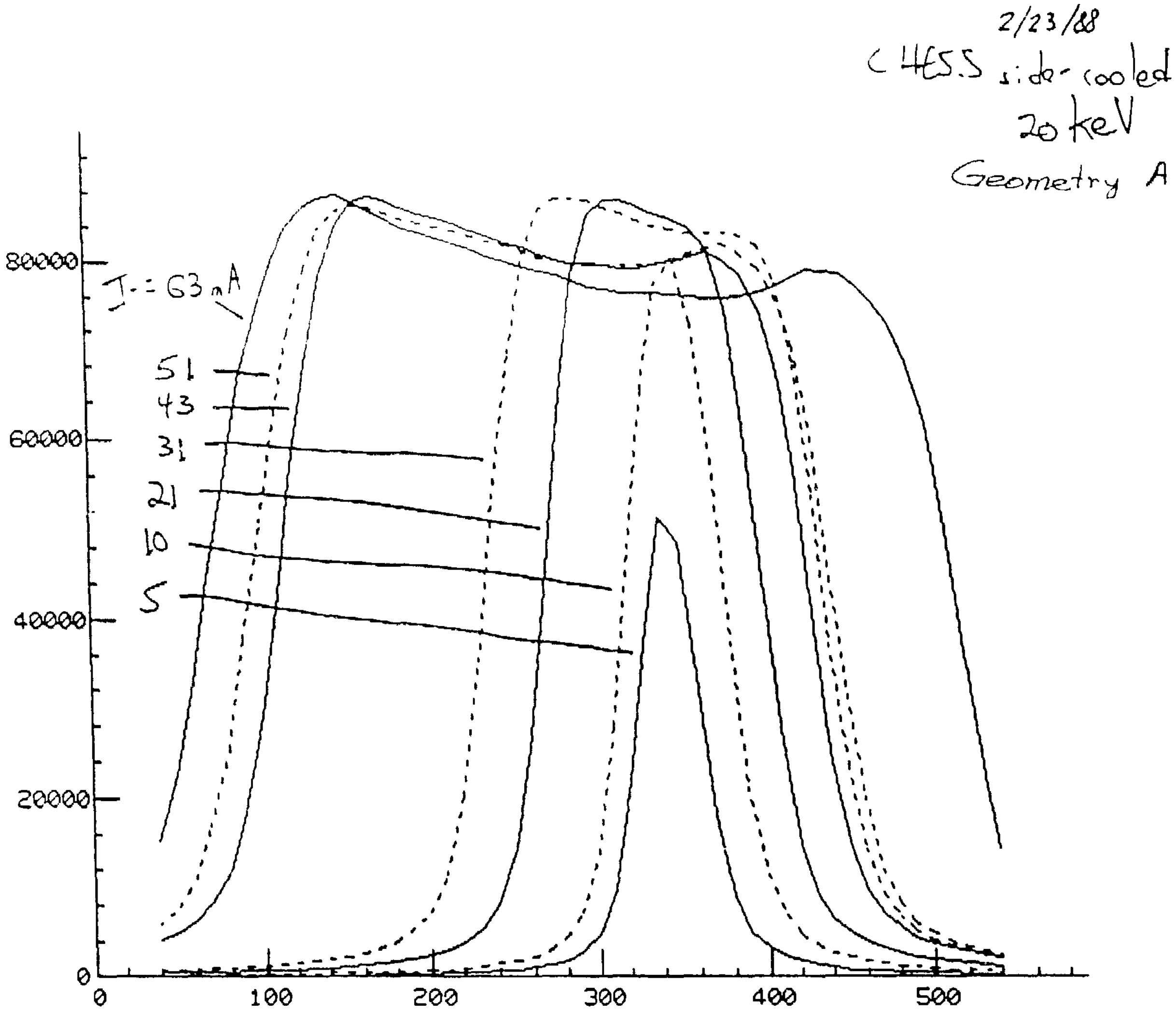
C. Testing at CHESS Wiggler
   February 1988

   Bob Smither and George Forster: Argonne
   Don Bilderback, Mike Bedzyk, K. Finkelstein, C. Henderson and J. White: Cornell
   Lony Berman, Peter Stefan and Tom Oversluizen: Brookhaven

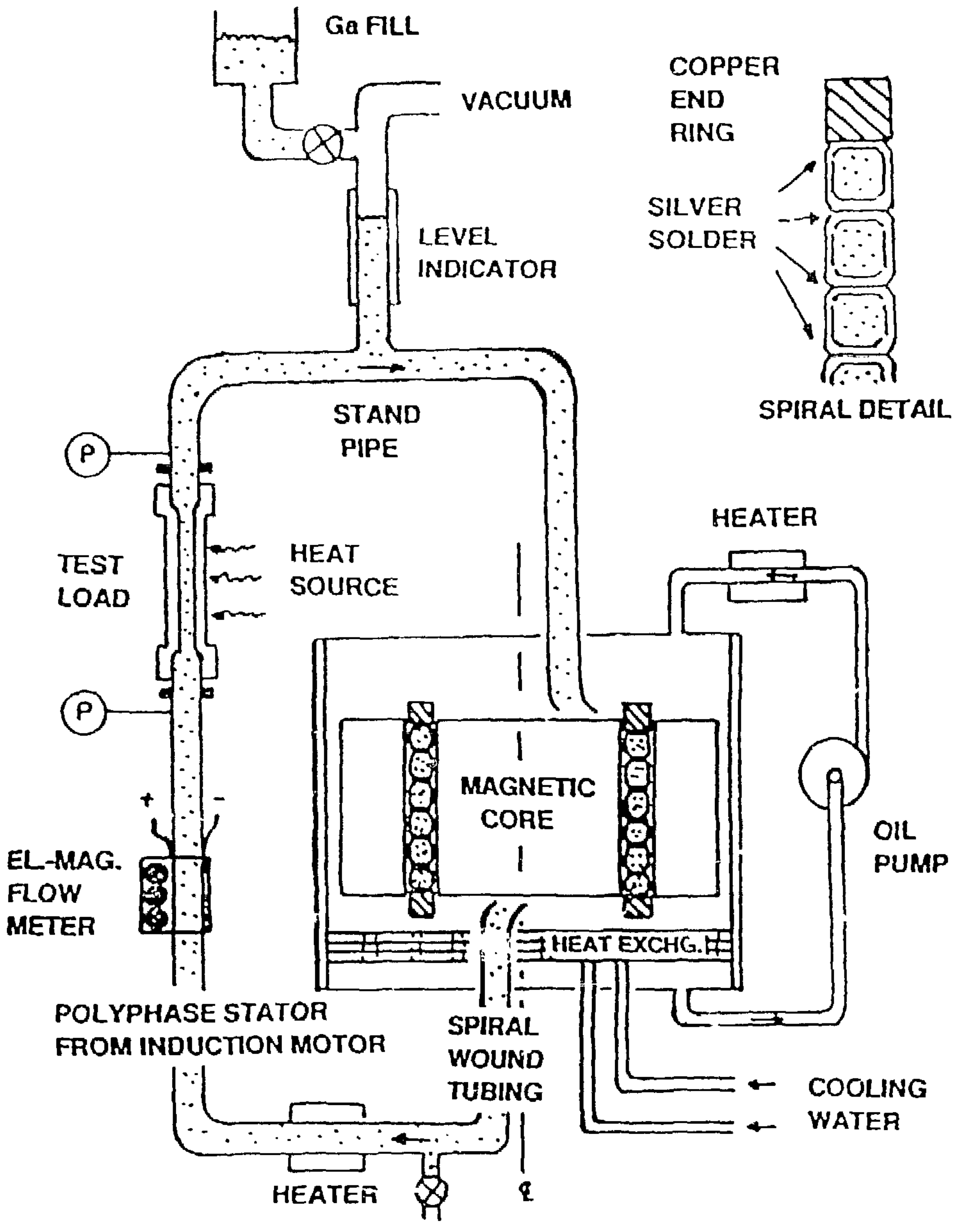
Geometry A

Standard CHESS Watercooled Geometry



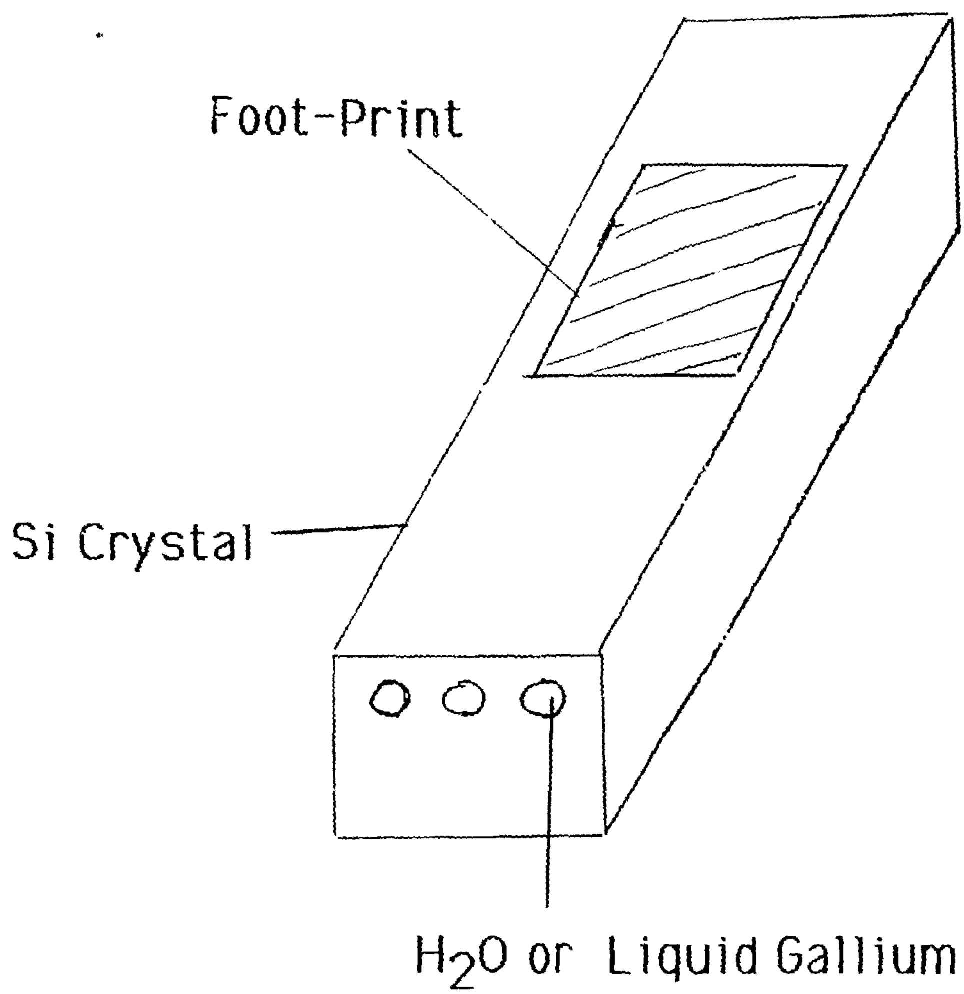


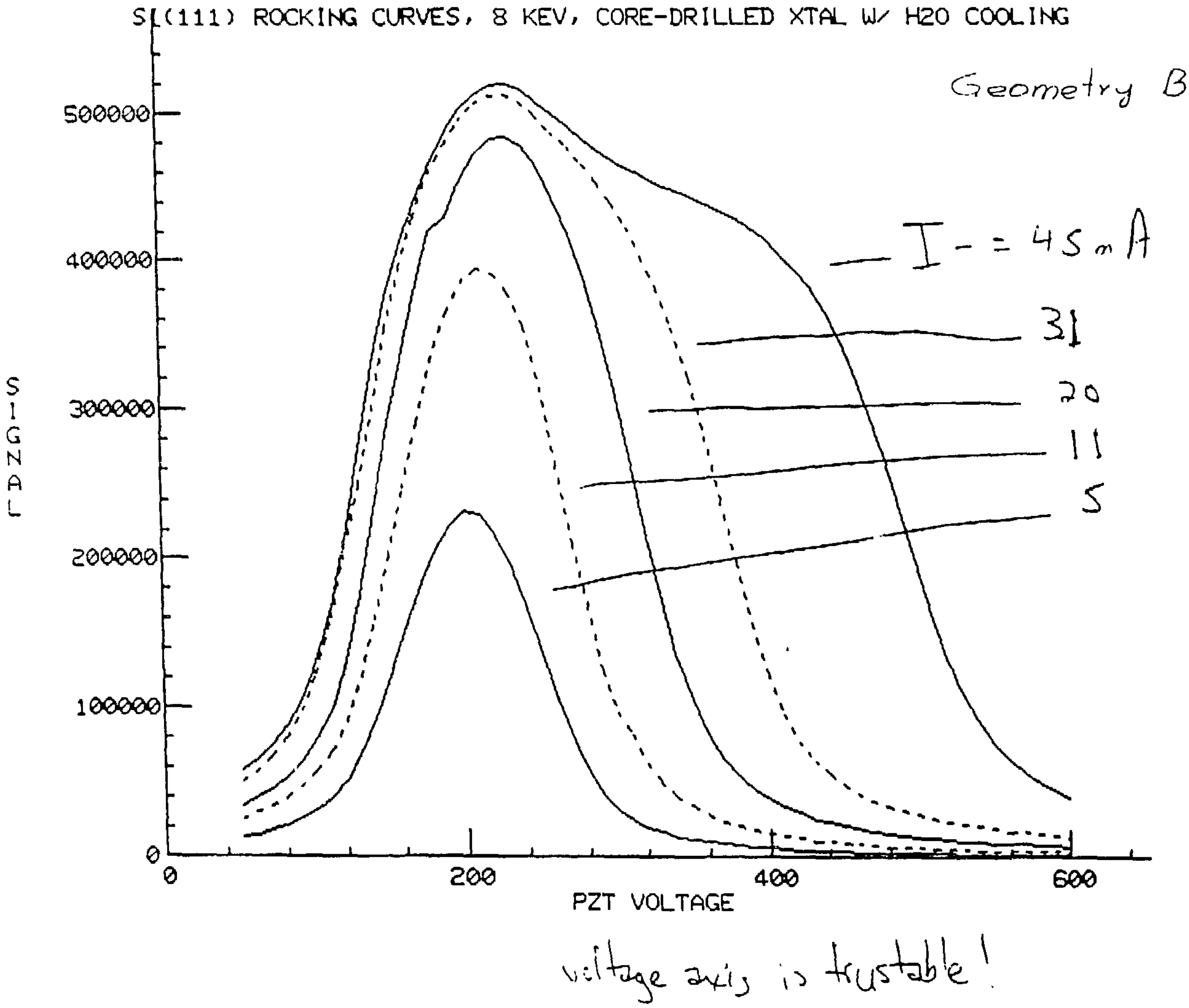
2/23/88
CHESS side-cooled
20 keV
Geometry A
I = 63 mA
51
43
31
21
10
5
80000
60000
40000
20000
0
0
100
200
300
400
500



Schematic drawing of the new gallium pump and its test system.

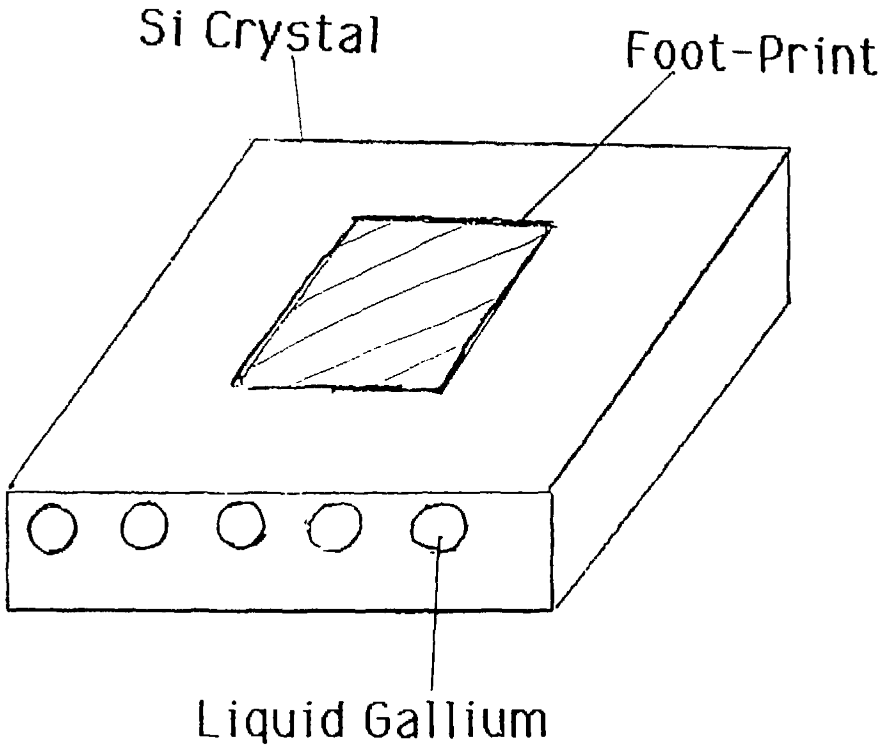
Geometry B
CHESS Standard Si Crystal

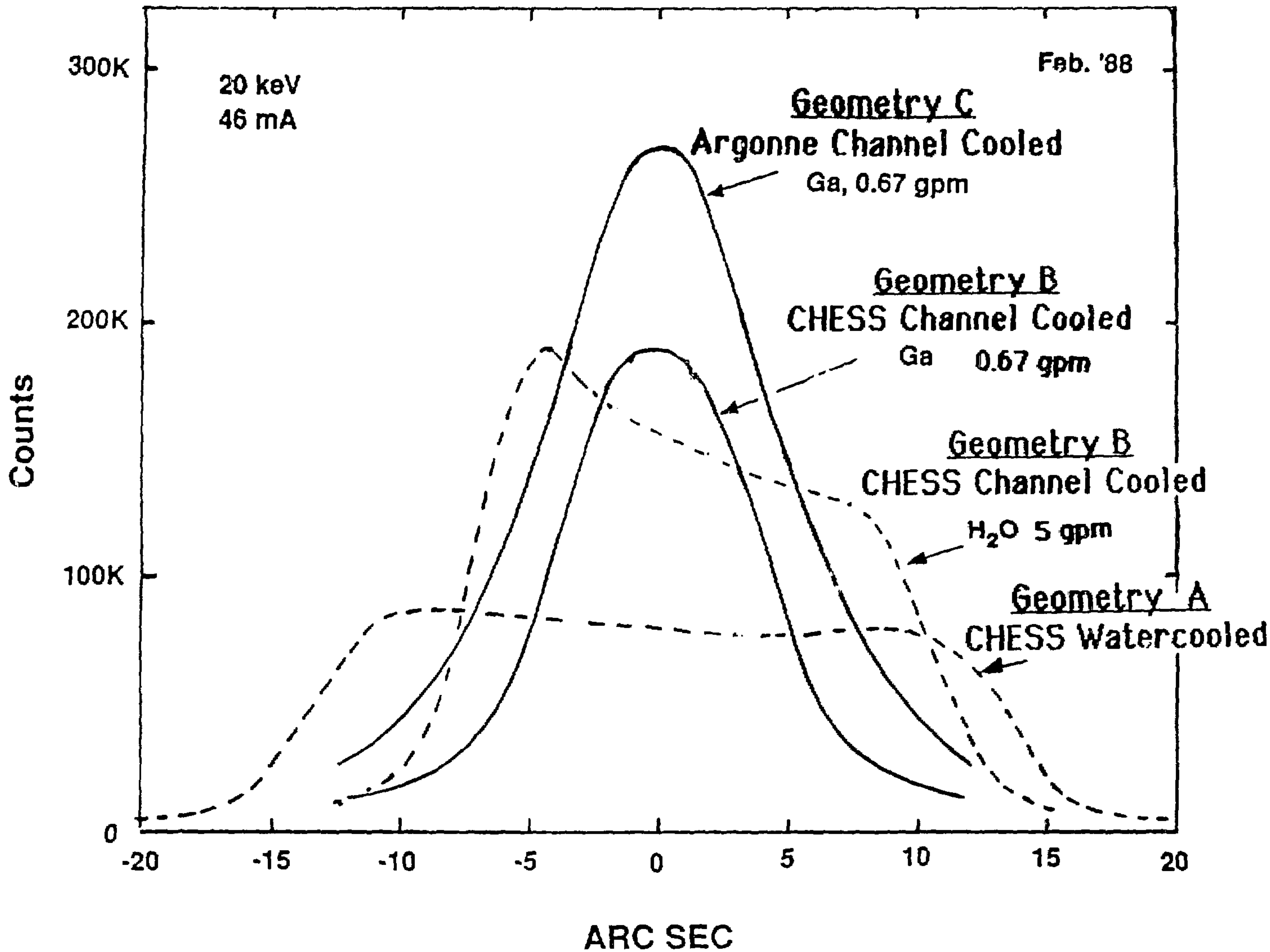




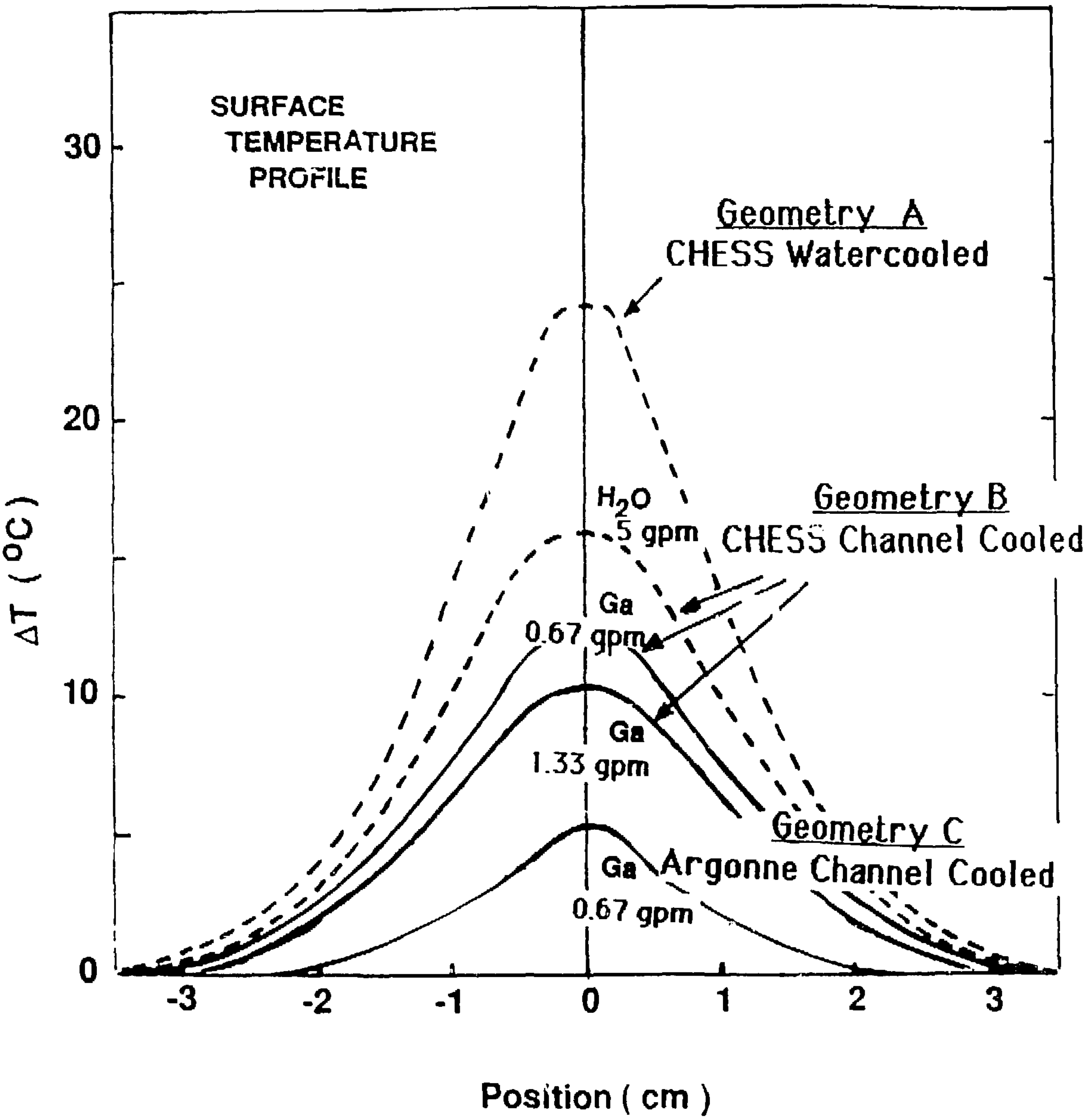
SI(111) ROCKING CURVES, 8 KEV, CORE-DRILLED XTAL W/ H2O COOLING
Geometry B
SIGNAL
500000
400000
300000
200000
100000
0
0
200
400
600
PZT VOLTAGE
I = 45 mA
31
20
11
5
voltage axis is trustable!

Geometry C
Argonne Optimized Si Crystal





20 keV
46 mA
Feb. '88
Geometry C
Argonne Channel Cooled
Ga, 0.67 gpm
Geometry B
CHESS Channel Cooled
Ga 0.67 gpm
Geometry B
CHESS Channel Cooled
H_2O 5 gpm
Geometry A
CHESS Watercooled
Counts
300K
200K
100K
0
-20
-15
-10
-5
0
5
10
15
20
ARC SEC



SURFACE TEMPERATURE PROFILE
Geometry A
CHESS Watercooled
Geometry B
CHESS Channel Cooled
Geometry C
Argonne Channel Cooled
H_2O
5 gpm
Ga
0.67 gpm
Ga
1.33 gpm
Ga
0.67 gpm
30
20
10
0
-3
-2
-1
0
1
2
3
ΔT (°C)
Position (cm)

APS CONVENTIONAL FACILITIES OVERVIEW*

Martin J. Knott
Argonne National Laboratory

Since the last users meeting and publication of the APS Conceptual Design Report, we've done considerable refinement on the design. Much of this work has been prompted by user requests through the conventional facilities subcommittee of the APSUO Steering Committee; some of it has also resulted from Department of Energy comments and from our own evaluation.

You've heard some references to the new user module design. We've also done some redesign on the central lab/office building and on the meeting facility, and of course we're working on an additional device, a positron accumulator ring. In addition, we have given considerable attention to the concrete shielding for the storage ring.

The design of the user lab/office modules was a particular concern of the Steering Committee. They wanted at least one laboratory and four office spaces for each beam line, and they wanted to reduce the travel distance between the labs and offices and the beam lines -- close to the experiment hall floor, but not so close as to be congested. We also thought it would be nice to allow for some custom design. And of course, an underlying goal was to try to hold the costs down.

We chose a 20 x 30 standard kind of laboratory space. This module here [see viewgraph], for example, has two labs and eight offices -- the arhitect's drawings indicate the range of customization possible. The common areas in the center are a conference room, a break area, restrooms, staff shop, and utilities. A parking lot is associated with each module. To summarize the changes: For the four units in the CDR design, we have a total of 16 laboratories. Lab space has been doubled and office space increased by half over the old design. We now have fewer clean rooms, but clean rooms did not seem to be a primary concern for the Committee. Gross square footage has increased to about half again the old value.

The central lab/office building has been redesigned in line with user recommendations and our own internal reviews. In light of the new user module design, we felt we could cut the number of user-specific labs in this building. We eliminated the Class 100 clean room to shorten the travel distance between the entrance and the floor; the Class 1000 clean room, for handling large objects, should be adequate for our needs. We also shortened the high-bay and machine-shop areas. But what really made the building design more compact is that we took the entire three-story lab/office building, raised it by one floor, and put it on top of these labs [see viewgraph]. We are now able to

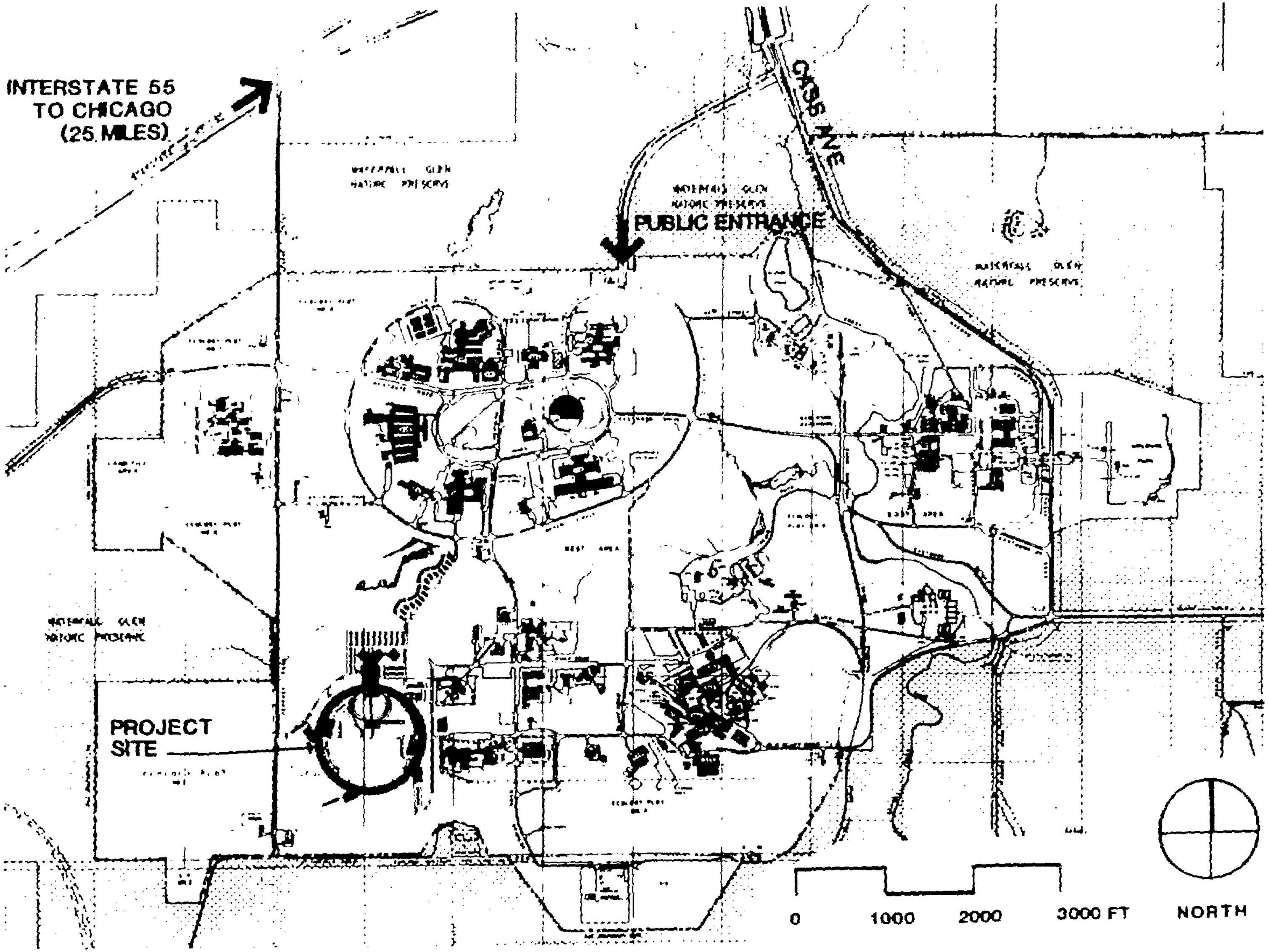
*The summary presented here is based on notes taken at the meeting; copies of viewgraphs were provided by the speaker.

provide a storage area that we can get into with a truck, rather than by elevator, and you can move large objects between the storage and the assembly areas.

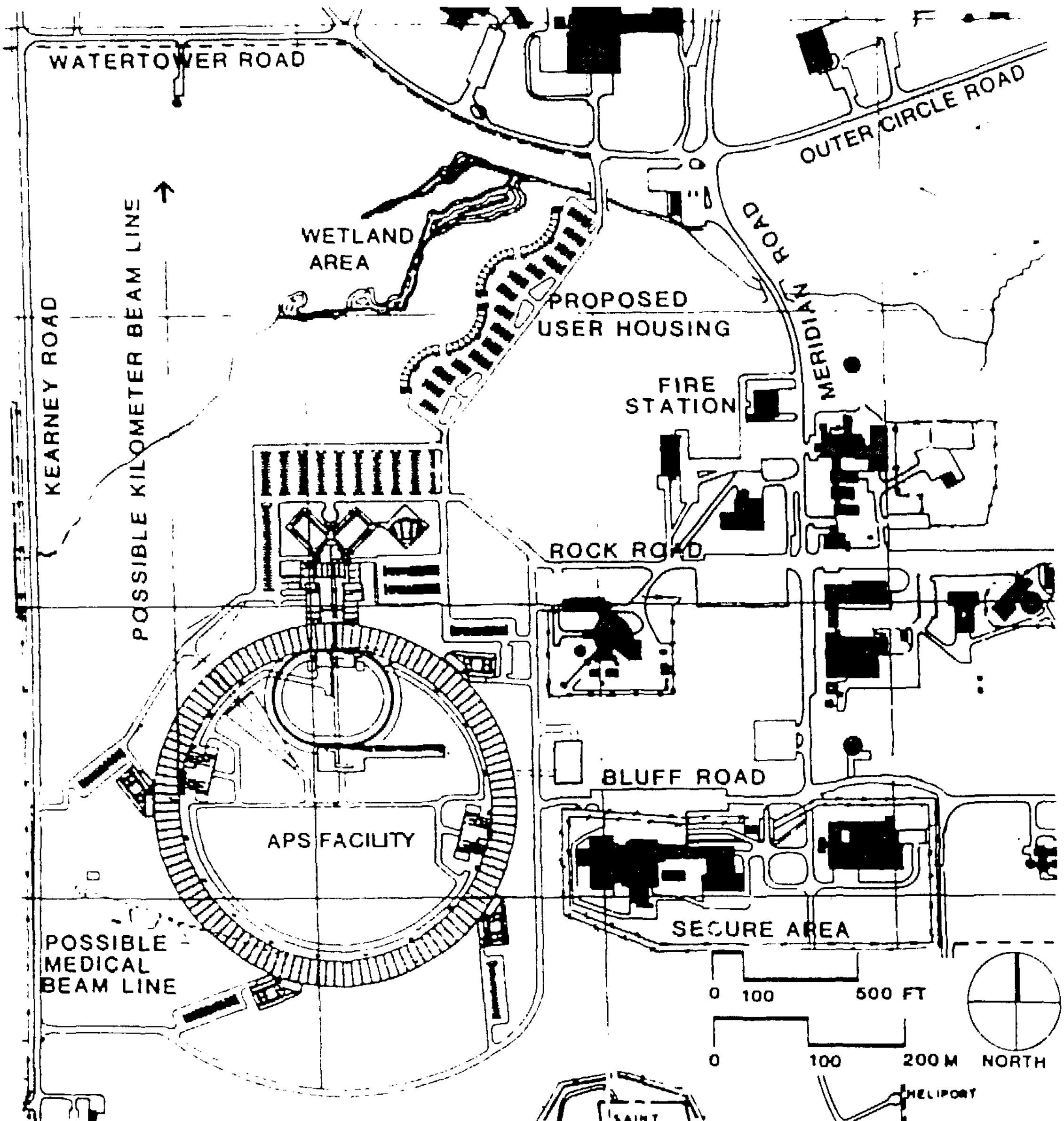
What used to be the auditorium is now the "Multi-Use Meeting Facility." This redesign was done at the prompting of the Department of Energy. The idea is to serve the user community better by providing the ability to handle a variety of meeting types, both large and small. For large meetings, this design provides a 600-seat capacity. There is room for several small meetings at 60 seats each, and we will be able to handle tables for tutorials and seminars, poster sessions, maybe catered banquets. The floor area can be divided up into halves, quarters, and even eighths to furnish this multi-use space. Soundproof walls can be brought across in two directions. The design is a bit complicated, in terms of making sure all these areas have doors and power and other necessities, but we feel it's a much more usable, flexible space than we had originally.

The ratchet-wall redesign effort was prompted by users' concern over how much beam-line space they would have available to them on the experiment hall floor. In the ideal storage ring, the beam line would begin at the source point. But in this design, as in any lattice, the beam takes a while to emerge from the lattice. So the users wanted us to move the ratchet wall toward the machine in order to bring the first optics closer to the source point. Of course, we still had to maintain radiation shielding quality and accommodate any front-end devices required, which have to be within the shield, but we managed to provide over six meters. The beam-line length on the floor was increased by 6.1 m for insertion devices and 6.4 m for bending magnets.

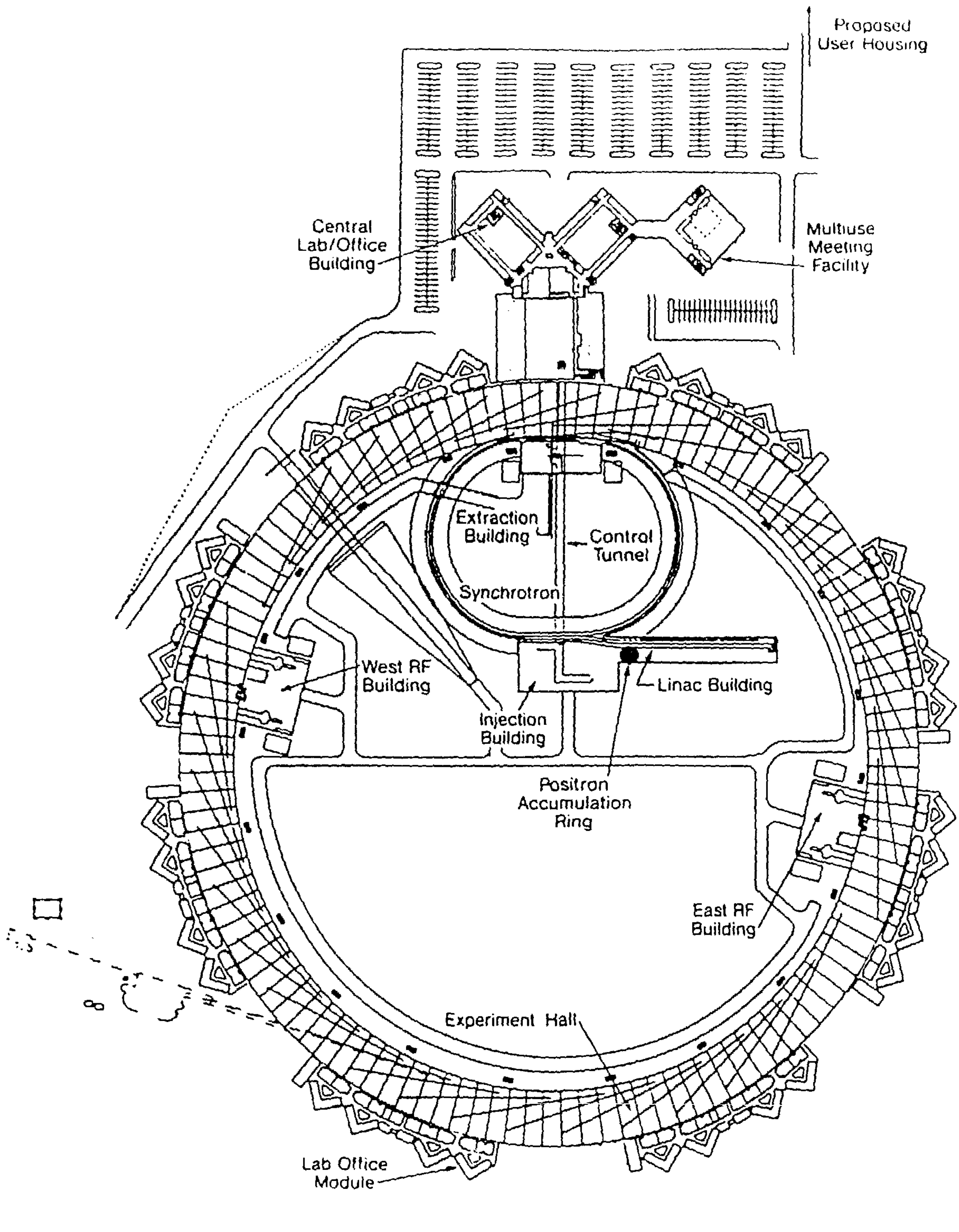
The first thing we did was switch to heavy concrete for the wall material, allowing us to decrease the thickness from 80 cm down to 56 cm. Also, we found that the front-end components could be put closer together and fit in a shorter length. The result was we gained more than six meters, and the clearances are the same as in the first design. You'll see this in the mock-up. At present only the inside skin is modeled; perhaps later on we may model the outside skin and some beam-line components and see if this is really workable.



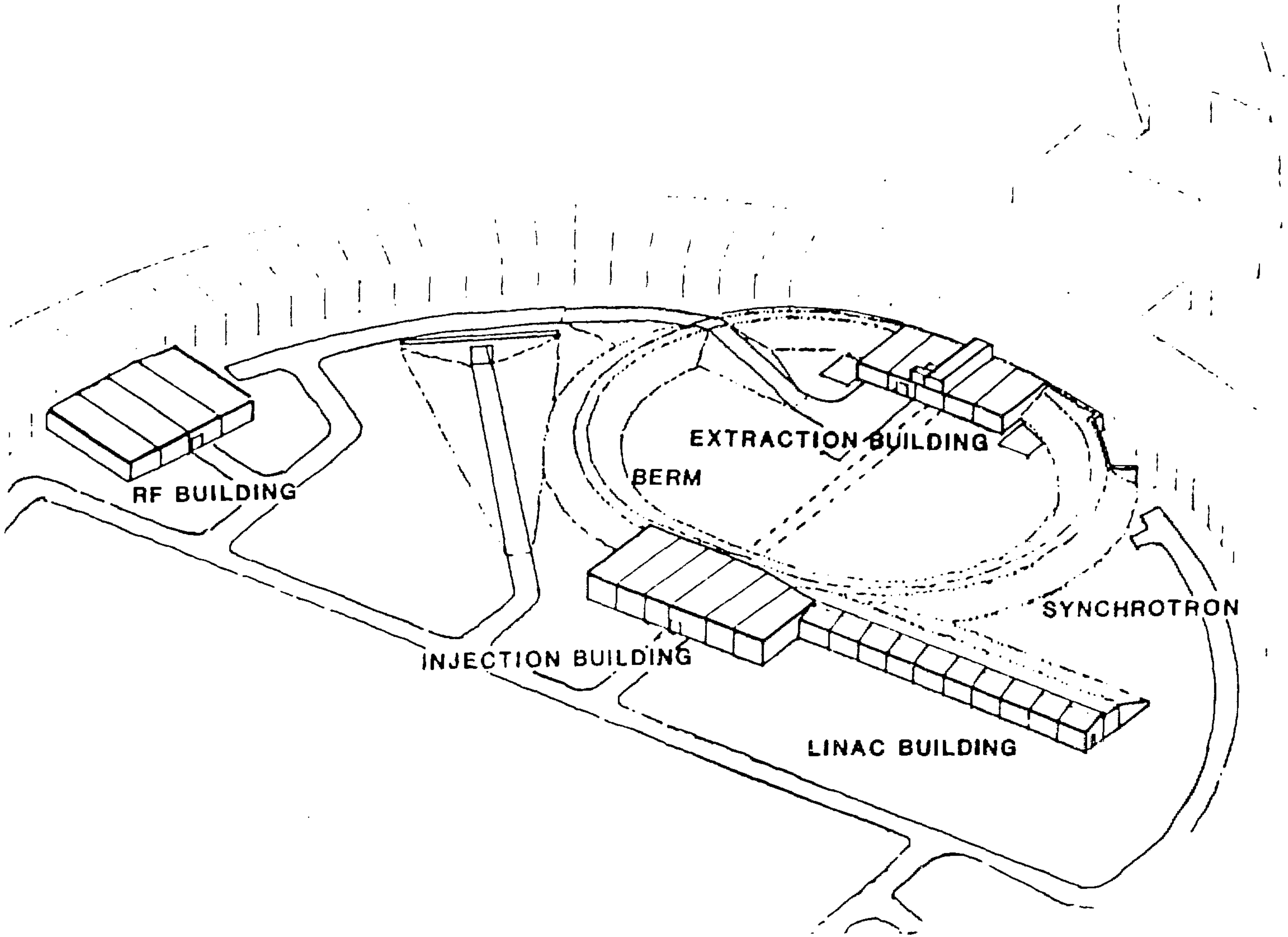
Argonne Site Plan



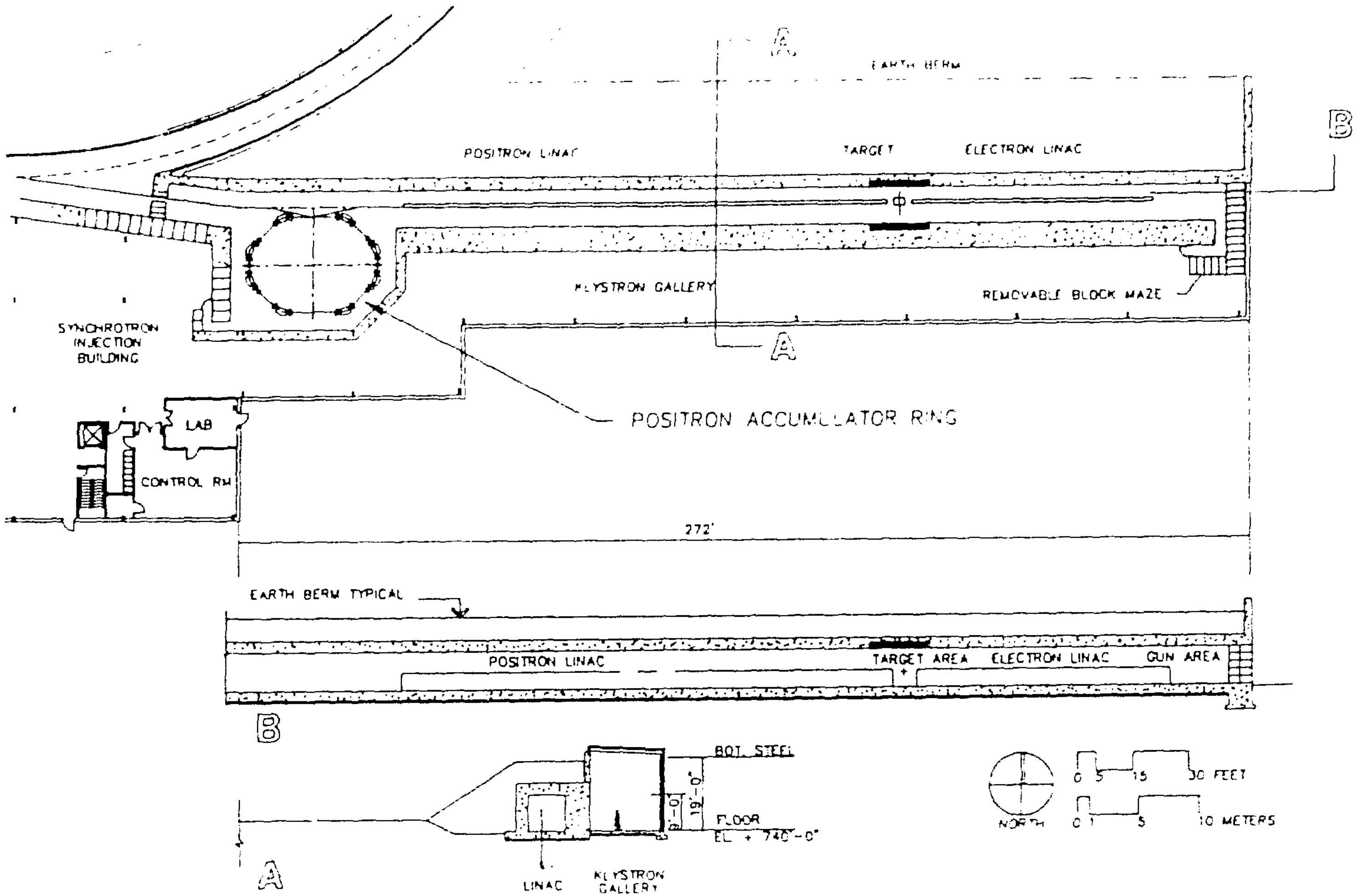
Project Area Plan



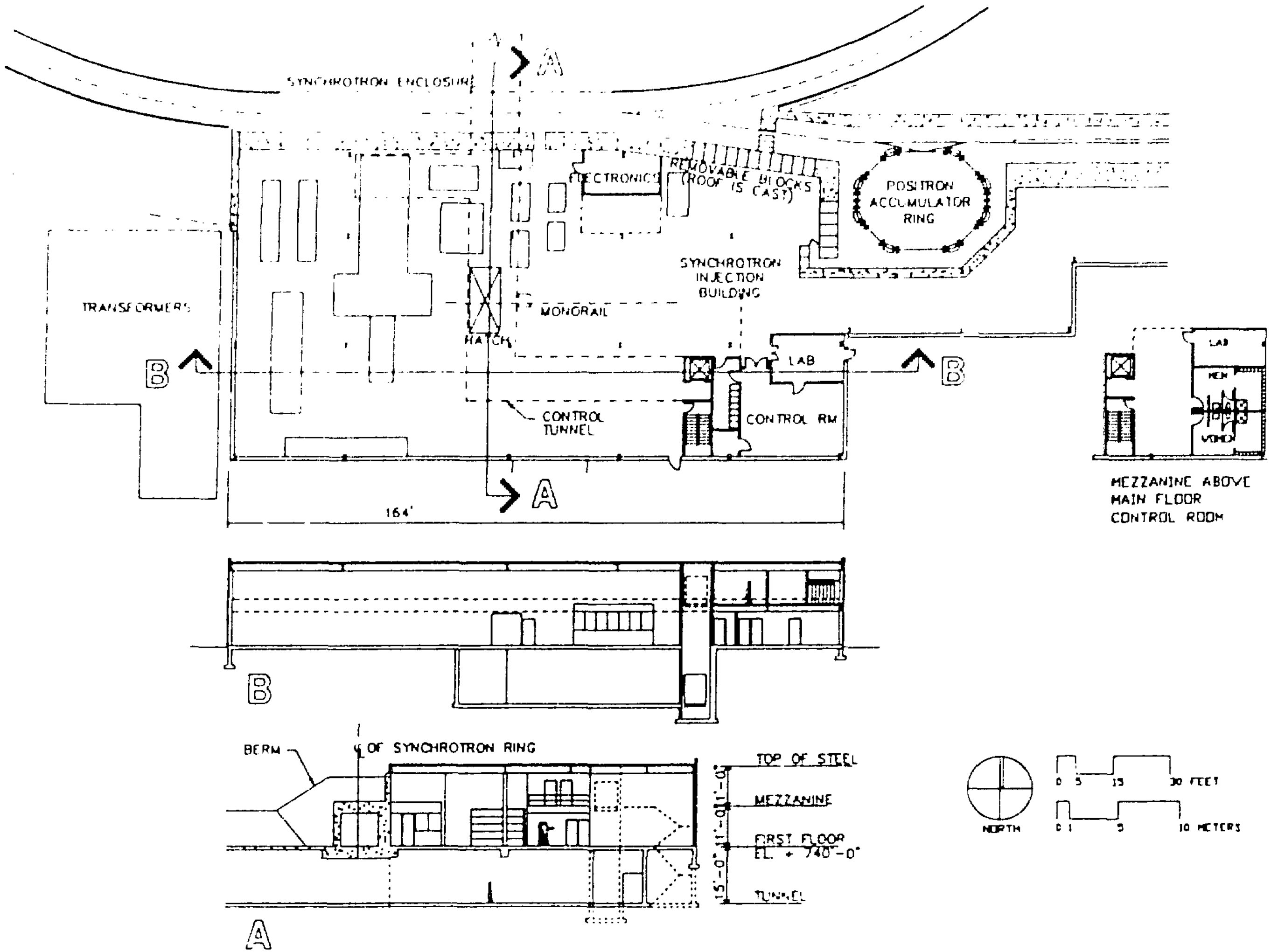
Project Site Plan



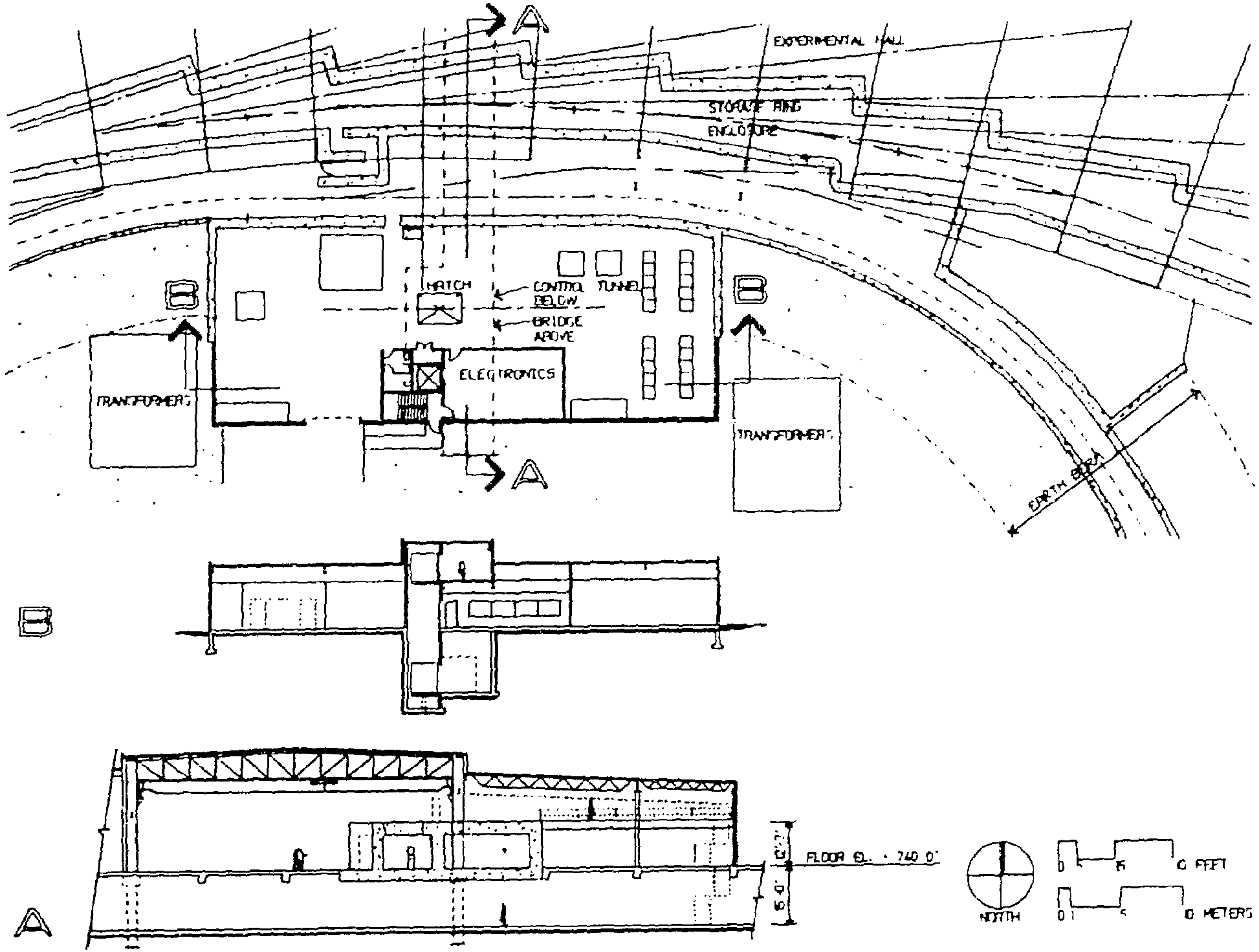
Infield Area



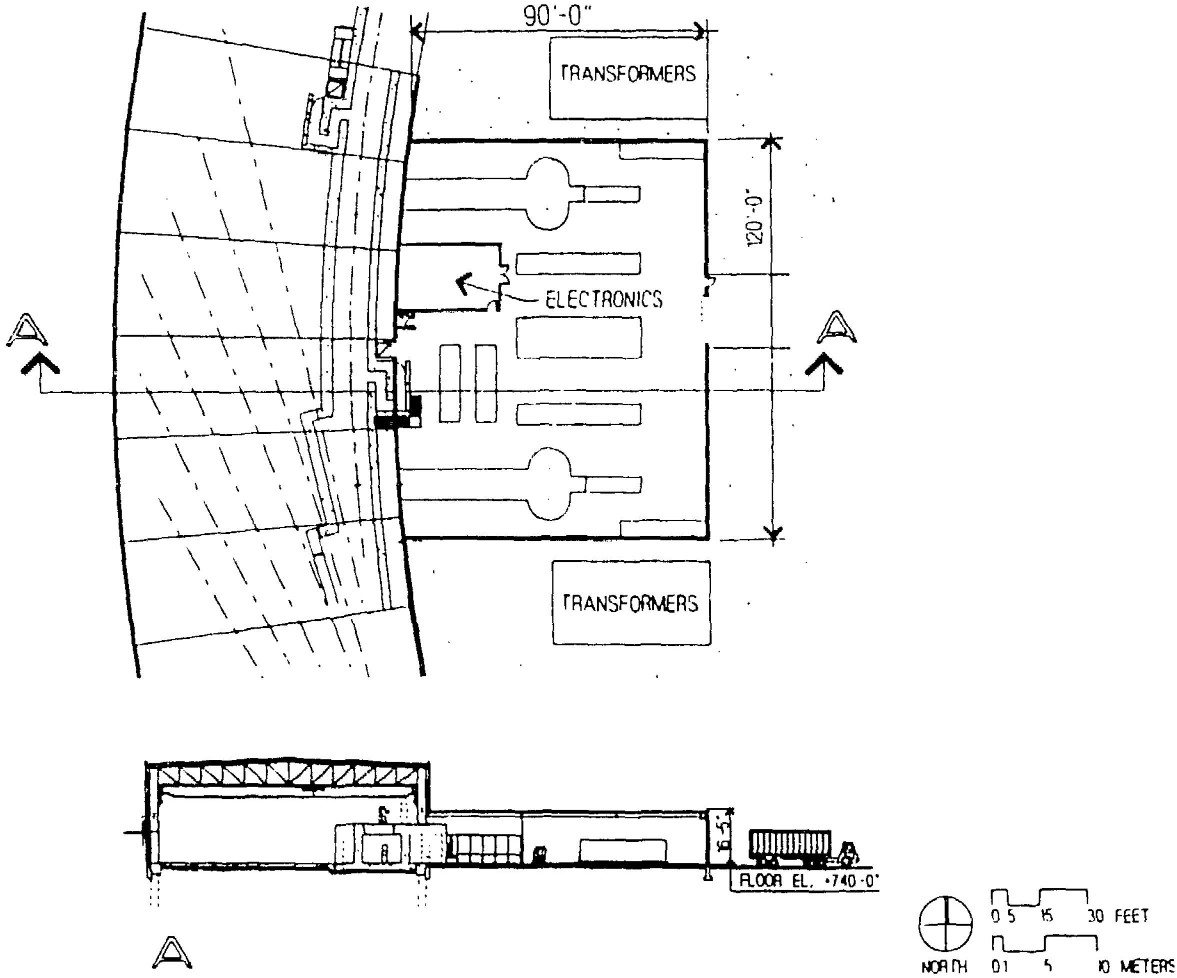
Linac Building



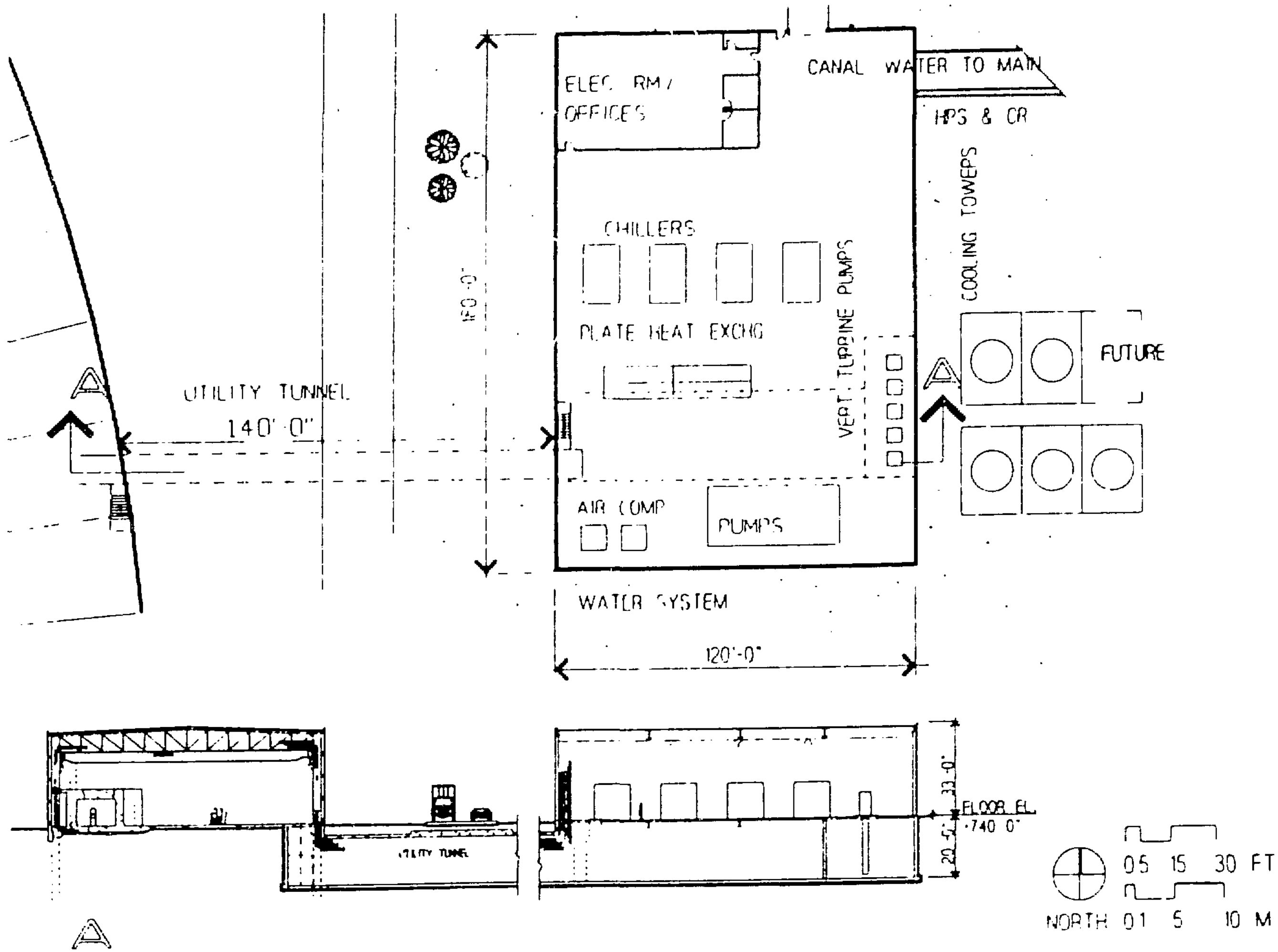
Synchrotron Injection Building



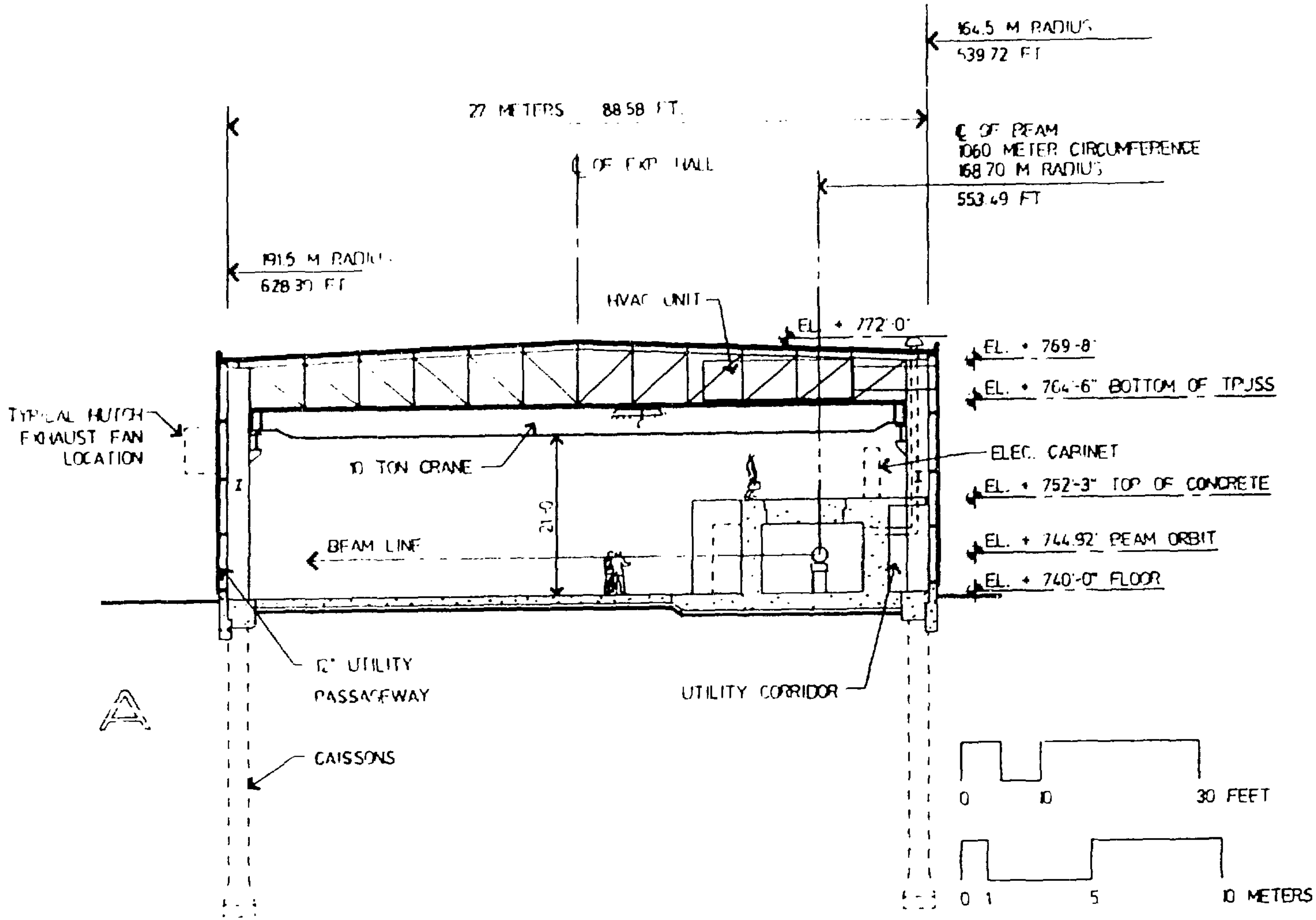
Synchrotron Extraction Building


90'-0"
TRANSFORMERS
120'-0"
ELECTRONICS
TRANSFORMERS
16'-5"
FLOOR EL. +740'-0"
NORTH
0 5 15 30 FEET
0 1 5 10 METERS

RF Building



Utility Building



Experiment Hall Section

RATCHET-WALL

DESIGN EFFORT

Objectives:

- Move ratchet-wall and first optics closer to source point.

- Maintain radiation shielding quality.

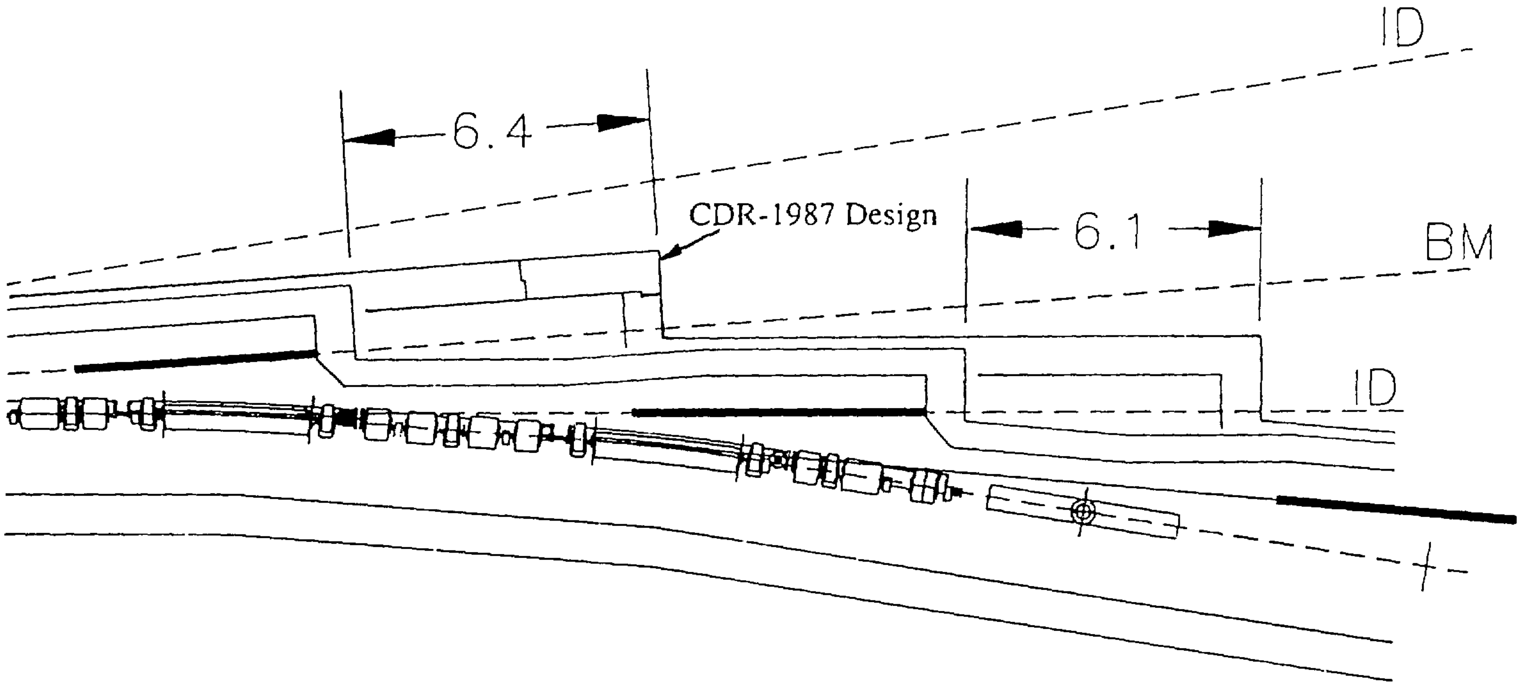
- Accommodate frontend devices.

Results:

- ID beamline length-on-floor increased by 6.1 meters.

- BM beamline length-on-floor increased by 6.4 meters.

- All important clearances maintained.



Ratchet-Wall Design Change

APS BEAMLINE

DIMENSION SUMMARY

(meters)

LONGITUDINAL	ID BEAM	BM BEAM
Source - to - frontend	23.1	21.7
Frontend length	6.1	5.0
Ratchet wall thickness	0.8	0.8
Ratchet wall - to - end	50.0	52.5
Total	80.0	80.0

TRANSVERSE	(BOTH)
Frontend centerline - to - wall	0.8
Beamline centerline - to - wall	0.2 (increasing to 0.5 in the first 4 m)
Beamline - to - beamline	2.3 (both emerged) 5.5 (at end)

USER LAB/OFFICE MODULE

DESIGN EFFORT

Objectives:

- Provide one (20' x 30') lab for each beamline.

- Provide four office spaces for each beamline.

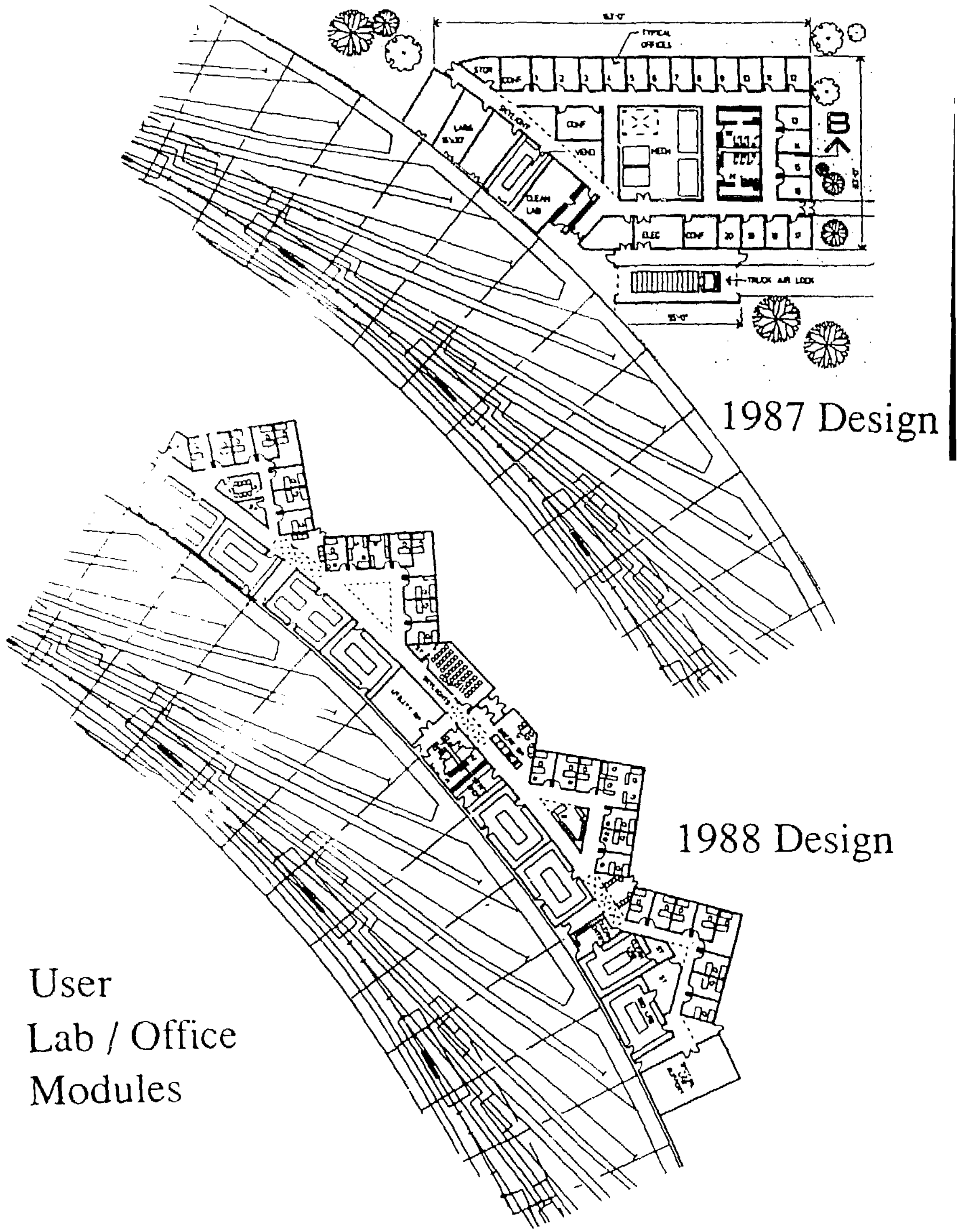
- Reduce travel distances from beamlines to labs, offices, and rest rooms.

- Keep office area separated from experimental floor congestion and traffic.

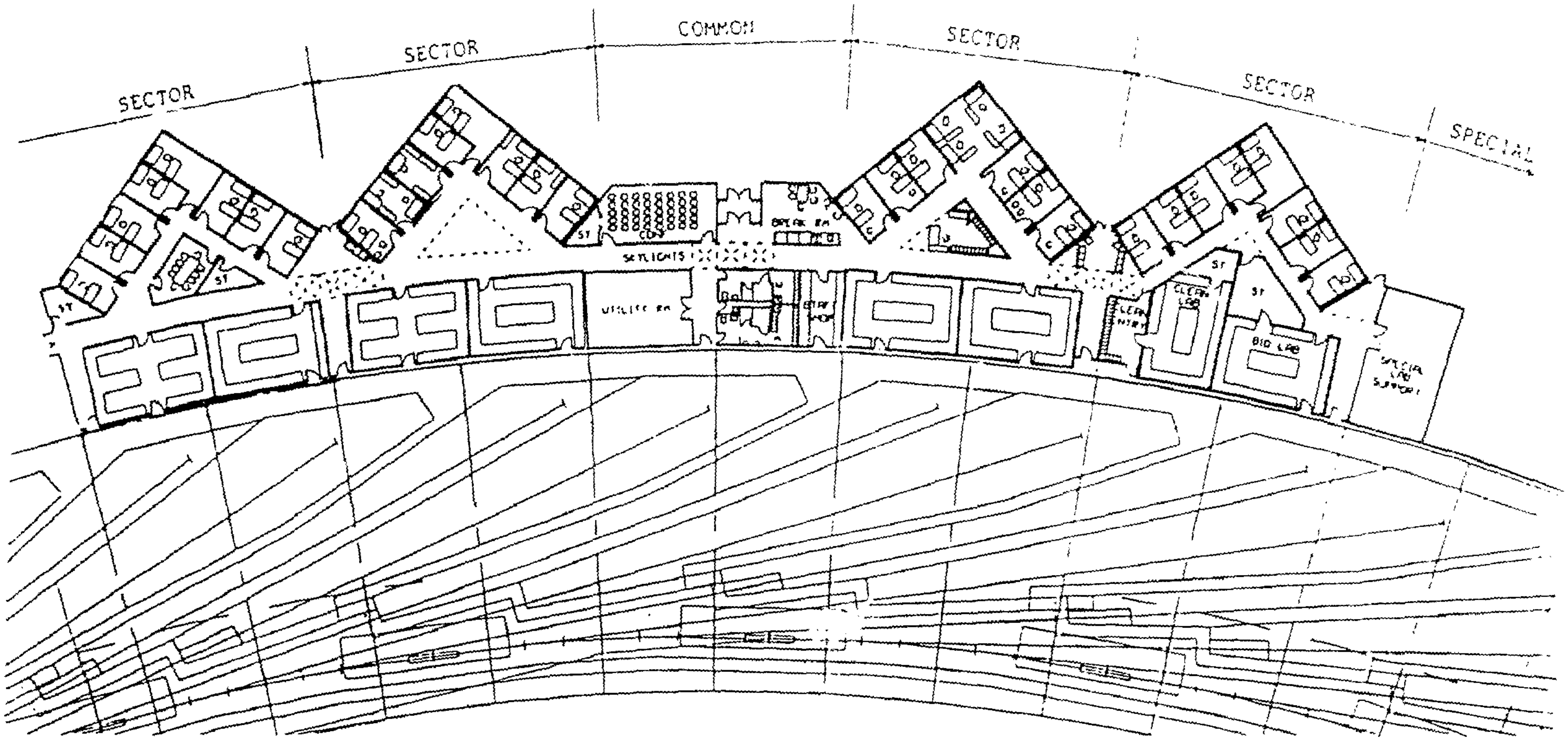
- Allow for some custom designs by users.

- Increase the number of common facilities:
  - Rest rooms / lockers
  - Kitchen / break rooms
  - Staff shops
  - Outside entrances
  - Conference rooms

- Hold total cost constant if possible.


1987 Design
1988 Design
User
Lab / Office
Modules

User Lab / Office Module - 1988 Design



USER MODULE

DESIGN CHANGE SUMMARY

PARAMETER	CDR-1987 DESIGN (4 units)	PRESENT DESIGN (4 units)	PRESENT DESIGN (8 units)
Laboratories	16	32	64
Offices	80	128	256
Clean rooms (or other special)	4	2	4
Staff shops	0	4	8
Rest / locker rooms	4	4	8
Large conference	0	4	8
Kitchens	0	4	8
Truck air-locks	4	2	4
Gross area (sq. ft.)	54.4K	76. K	152.K

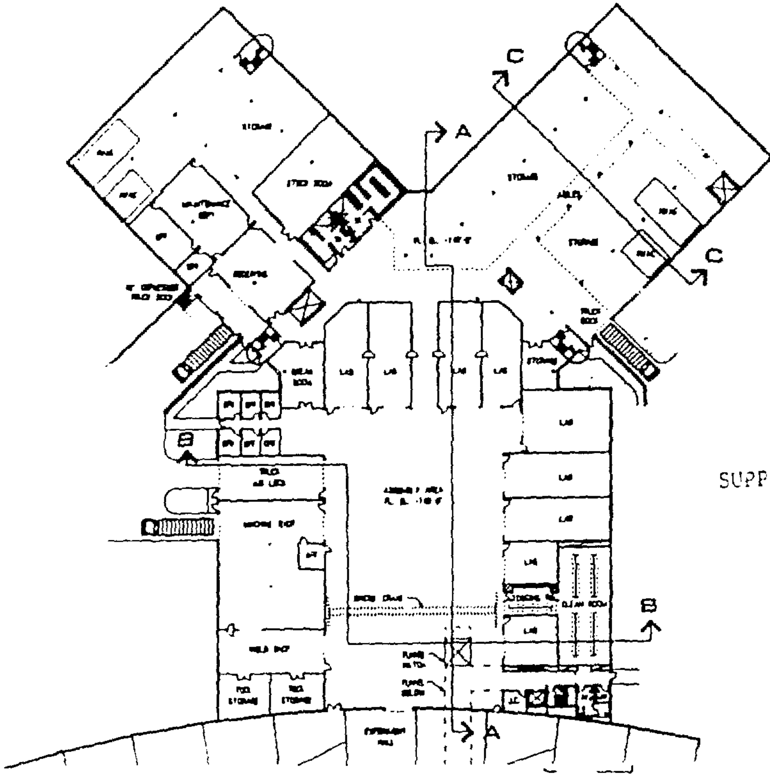
CENTRAL LAB/OFFICE BUILDING

DESIGN EFFORT

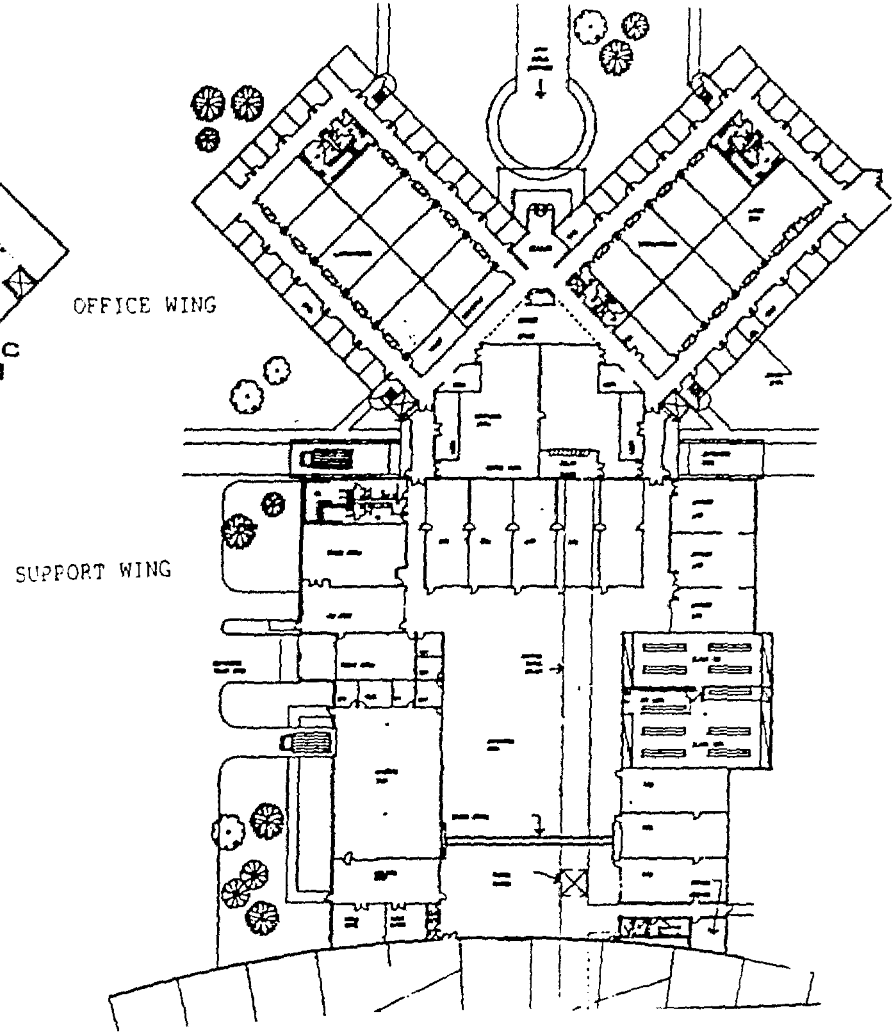
Objectives:

- Reduce experimental-support lab count in light of new user module design.
- Shorten travel distance from the entrance to the experimental floor.
- Eliminate Class-100 clean room (retain Class-1000 clean room).
- Provide path for staff and visitors which avoids high-bay assembly area.
- Make other visitor provisions if possible.
- Retain all adjacencies between various types of areas.
- Reduce cost (in light of new user module design).

1988 Design



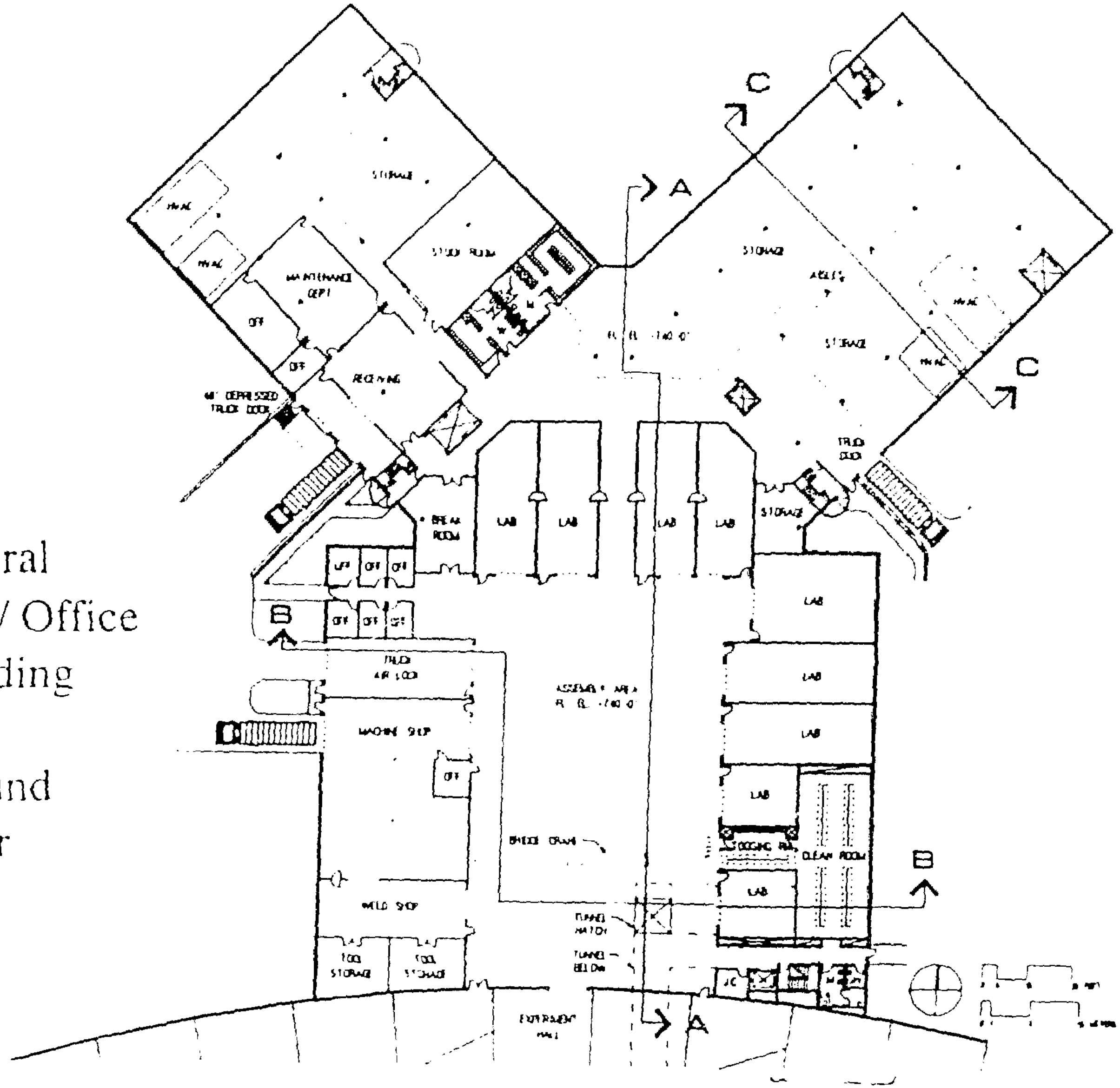
Central Lab / Office Building



1987 Design

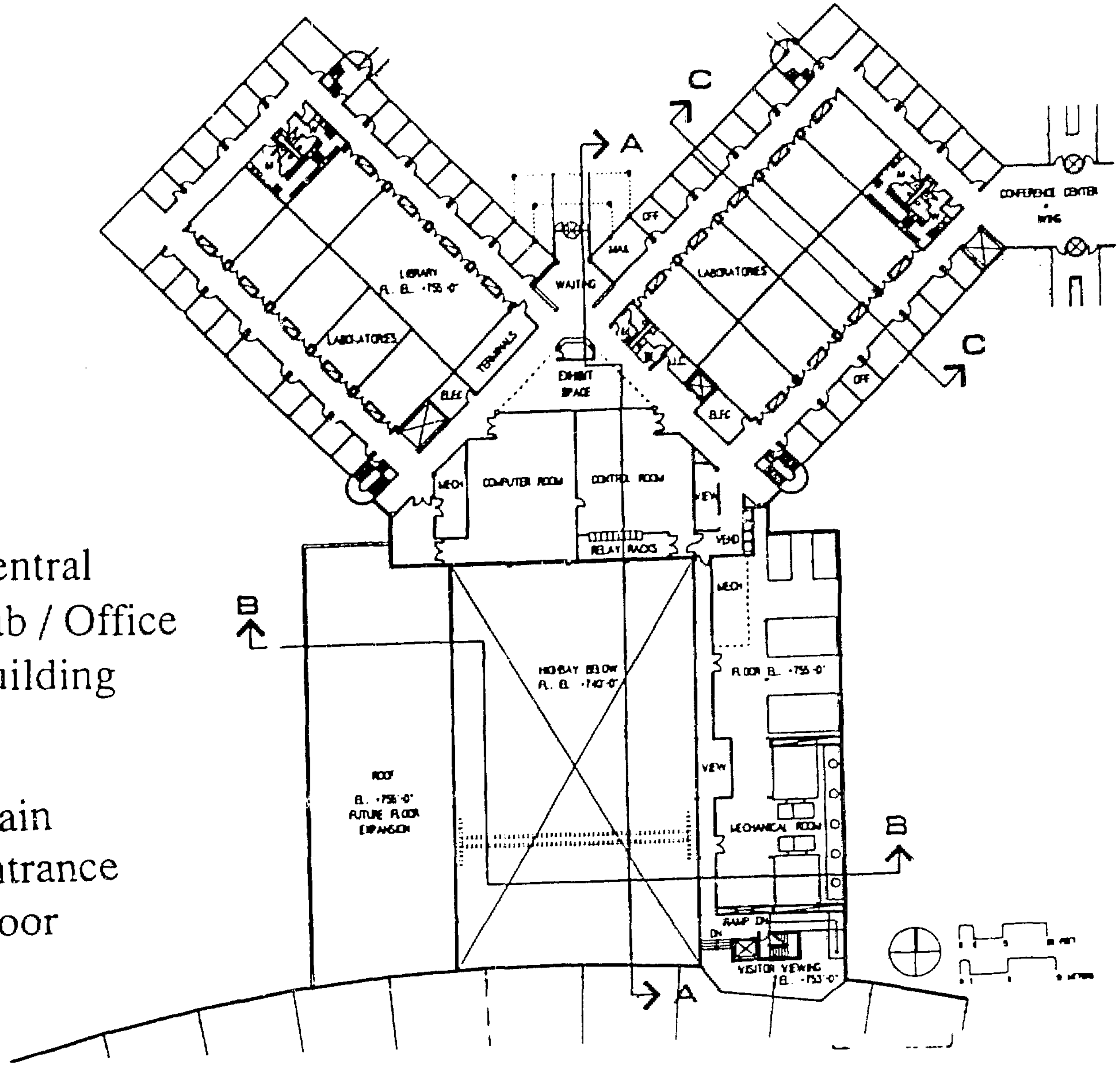
Central
Lab / Office
Building

Ground
Floor



Central
Lab / Office
Building

Main
Entrance
Floor



AUDITORIUM/MEETING FACILITY

DESIGN EFFORT

Objectives:

- Serve the APS community by accommodating:
  - Large and small meetings
  - Seminars and tutorials
  - Social and interactive functions
  - Several simultaneous functions

- Increase utility by accommodating:
  - One large (600 seat) meeting
  - Several small (60 seat) meetings
  - Seminar/tutorial tables
  - Poster sessions
  - Banquets (catered)
  - Vendor equipment demos

- Retain lobby interaction area.

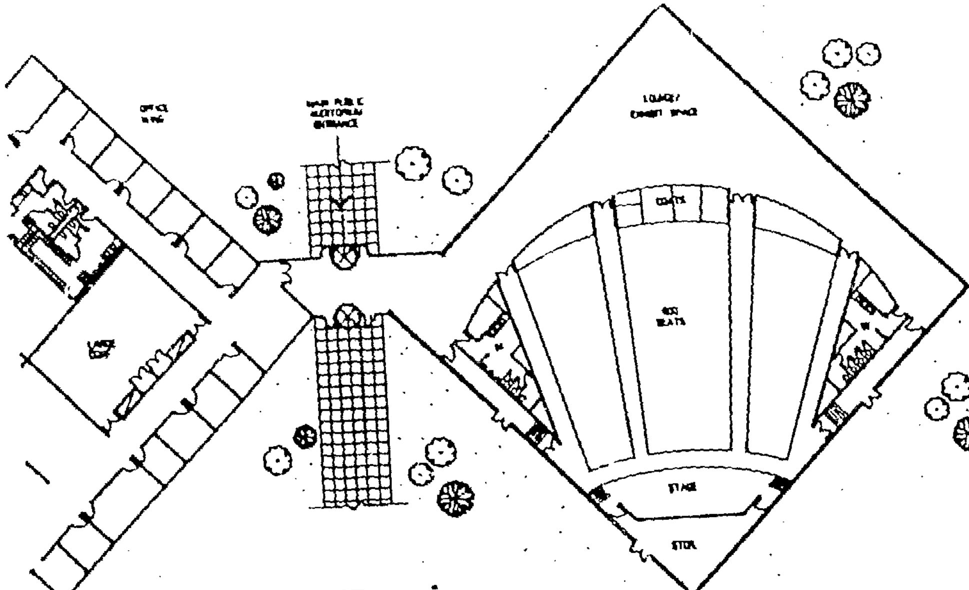
- Add small kitchen facility.

- Control sound for multiple programs.

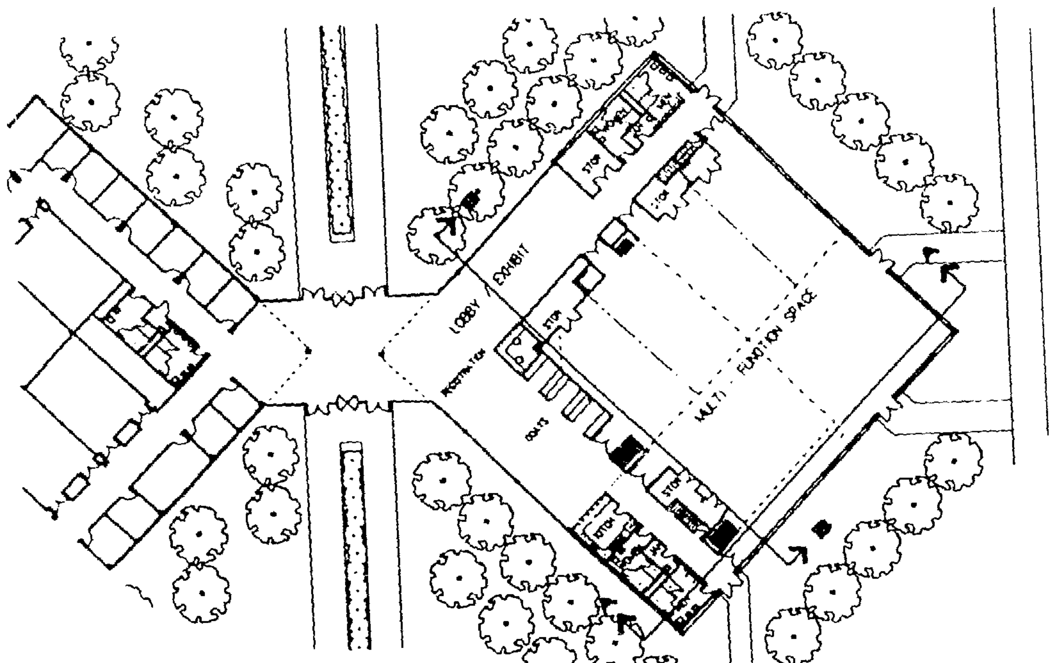
- Retain proximity to parking.

- Retain proximity to central lab/office building.

- Avoid cost increase.

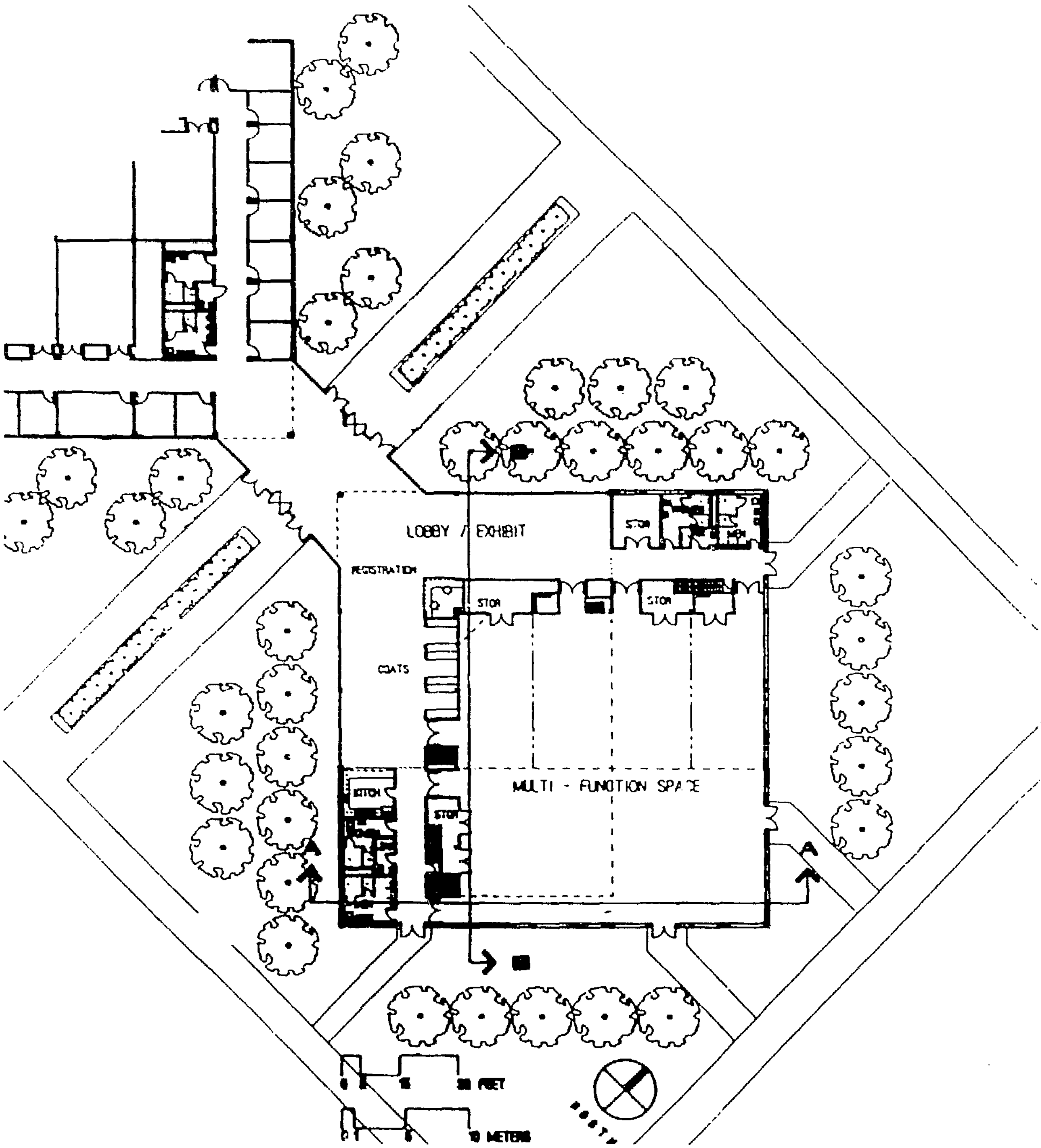


1987 Design

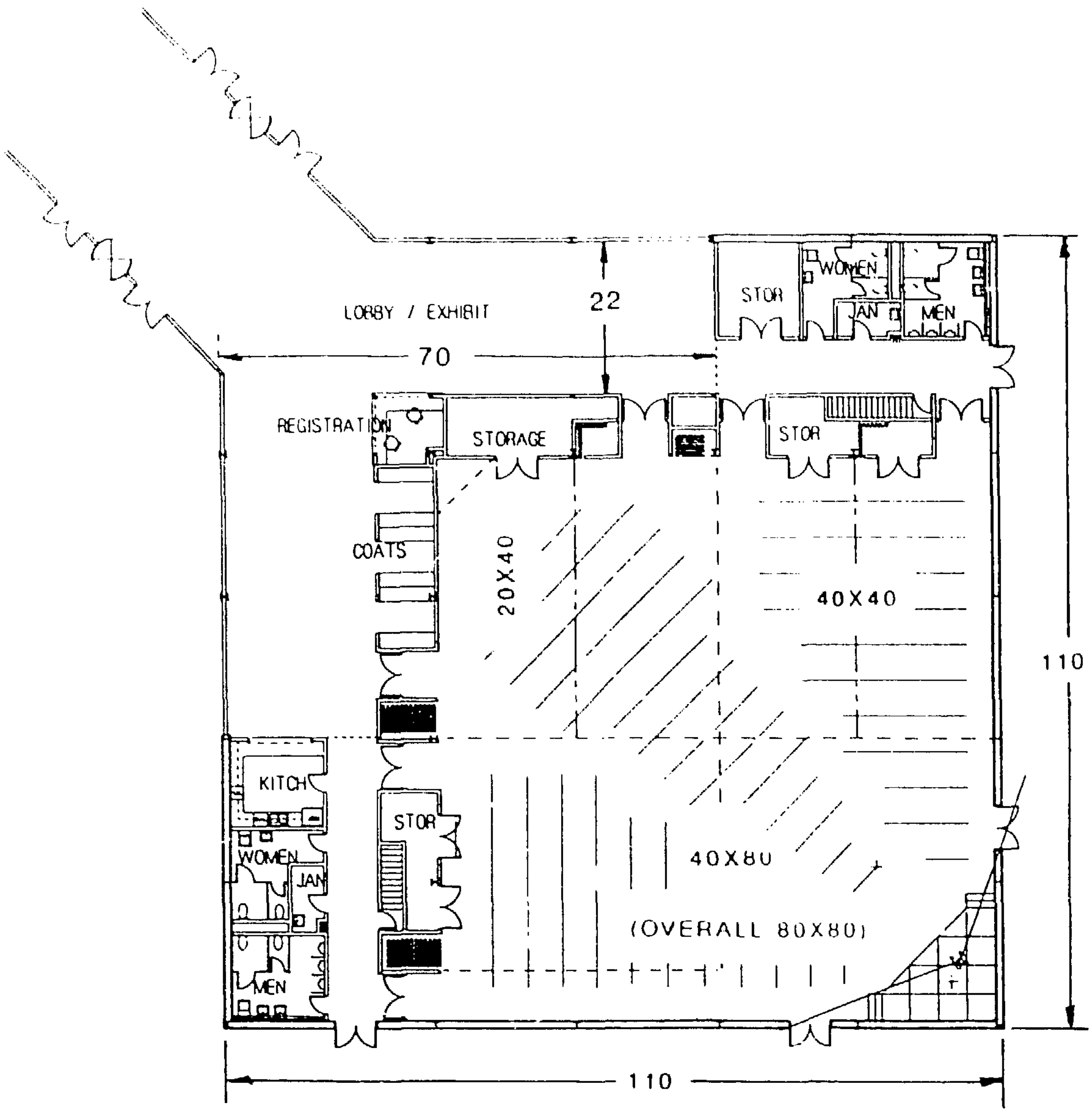


1988 Design

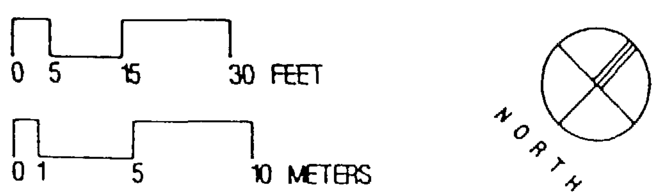
Auditorium / Meeting Facility

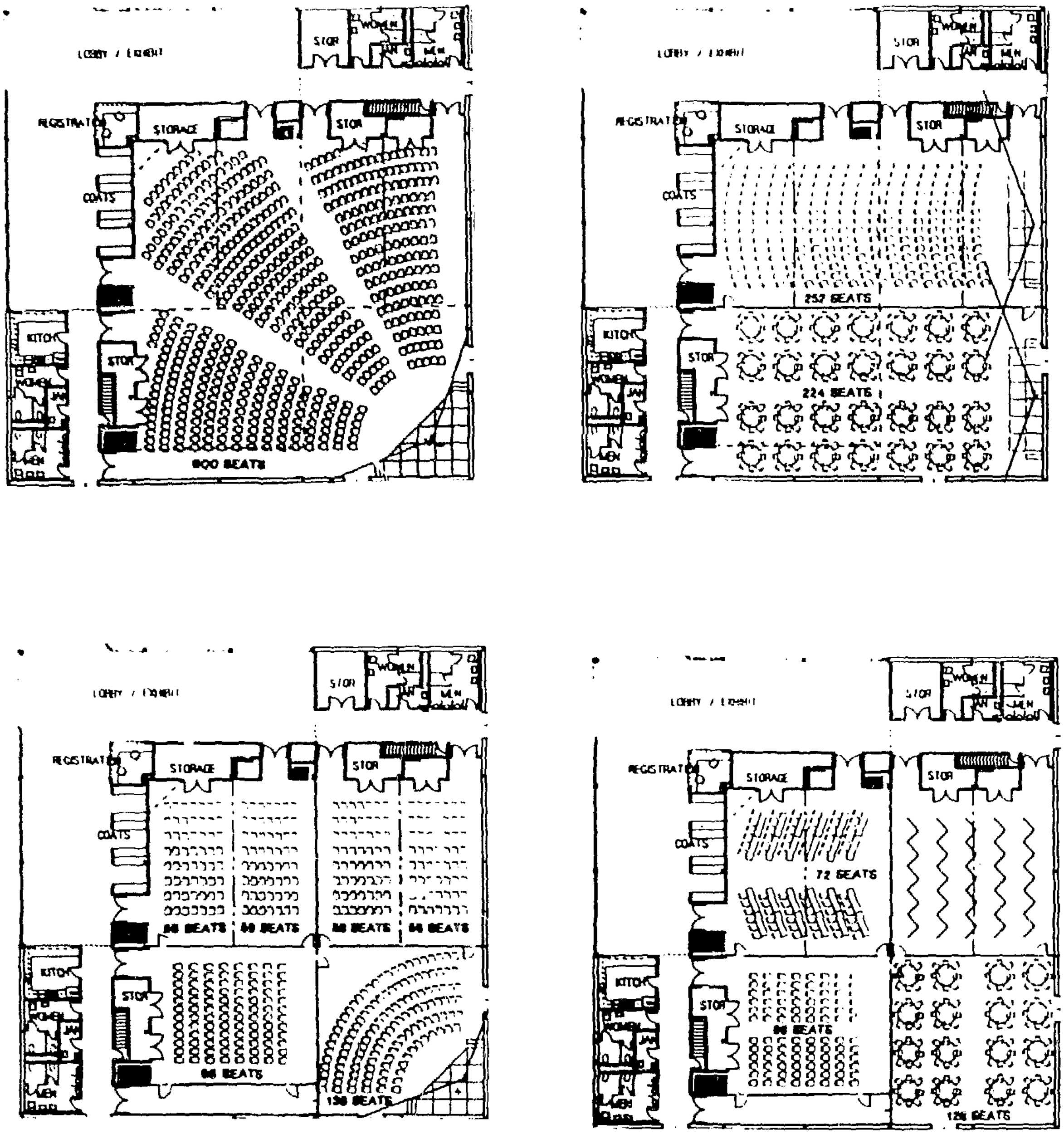


Multi-Use Meeting Facility Site Plan



Plan of Multi-Use Meeting Facility





Multi-Use Meeting Facility
Layout Examples

FRONTIERS IN SYNCHROTRON APPLICATIONS

MILLISECOND-RESOLUTION SCATTERING STUDIES OF PHASE-TRANSITION KINETICS*

G. Brian Stephenson
IBM Thomas J. Watson Research Center
Yorktown Heights, New York

ABSTRACT

A wide-bandpass monochromator and fast detector system at the IBM/MIT beam line X-20C at the National Synchrotron Light Source allow the collection of x-ray scattering patterns within milliseconds. The monochromator incorporates artificial multilayers rather than crystals and provides a flux of 1×10^{13} photons per second at 6 keV with an energy resolution of $\Delta E/E = 1.1 \times 10^{-2}$ fwhm. The detector system is based on a linear photodiode array. Using this beam line, we have carried out in-situ time-resolved scattering studies of the initial kinetics of crystallization, phase separation, and ordering at time scales orders of magnitude faster than previously possible for such nonrepetitive processes. These results have revealed a transient structure present during the rapid crystallization of amorphous $NiZr_2$ and the presence of nonlinearities during early-stage spinodal decomposition near the critical point in Al-Zn.

*The following abstract and copies of viewgraphs were provided by the speaker.

TIME-RESOLVED X-RAY SCATTERING STUDIES OF PHASE TRANSITION KINETICS

Collaborators:

K. Ludwig, J. Jordan-Sweet
IBM Research Division,
T. J. Watson Research Center

M. Sutton, J. Mainville, Y. Yang
McGill University
Dept. of Physics

I. Synchrotron Beamline for Time-Resolved X-ray Scattering

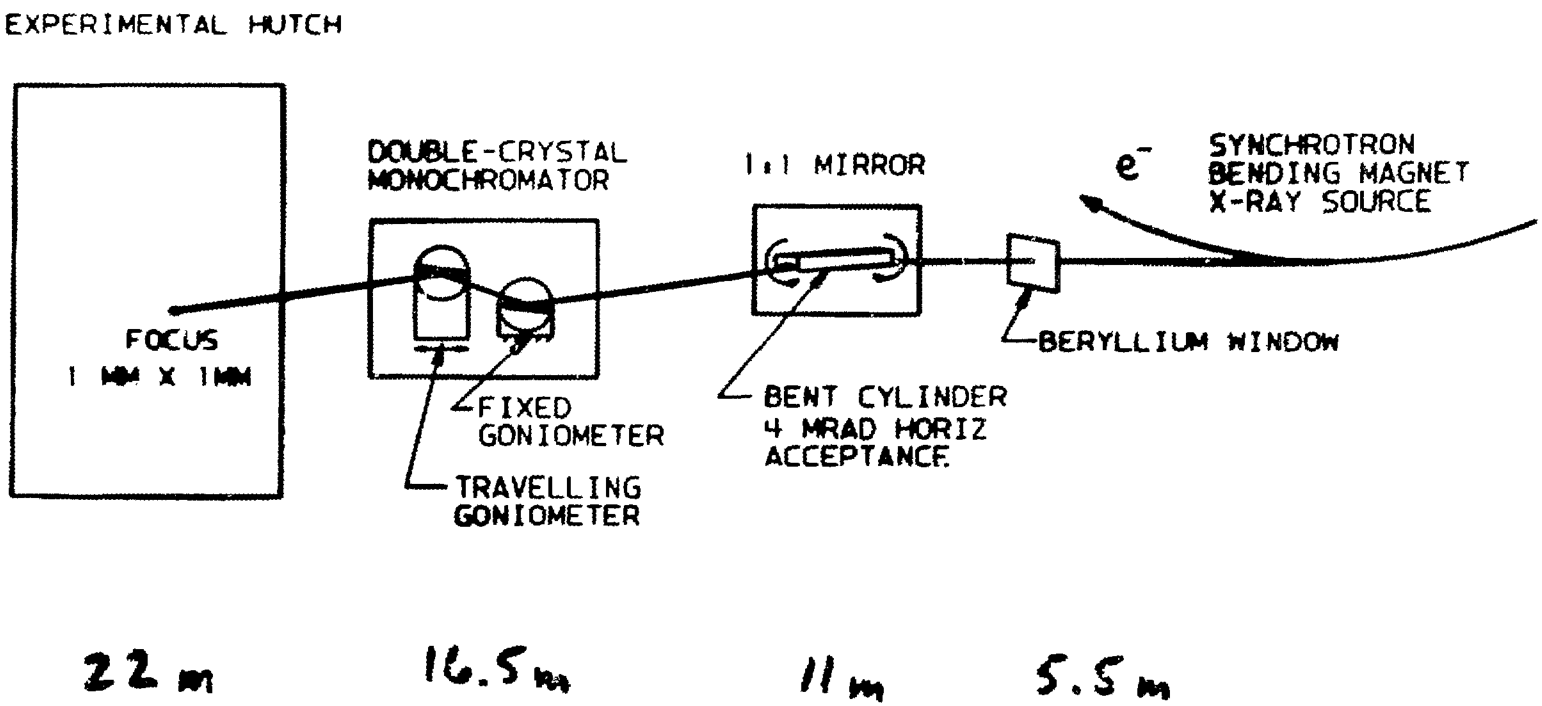
II. Studies of Phase Transition Kinetics

→ • Crystallization of Amorphous $NiZr_2$

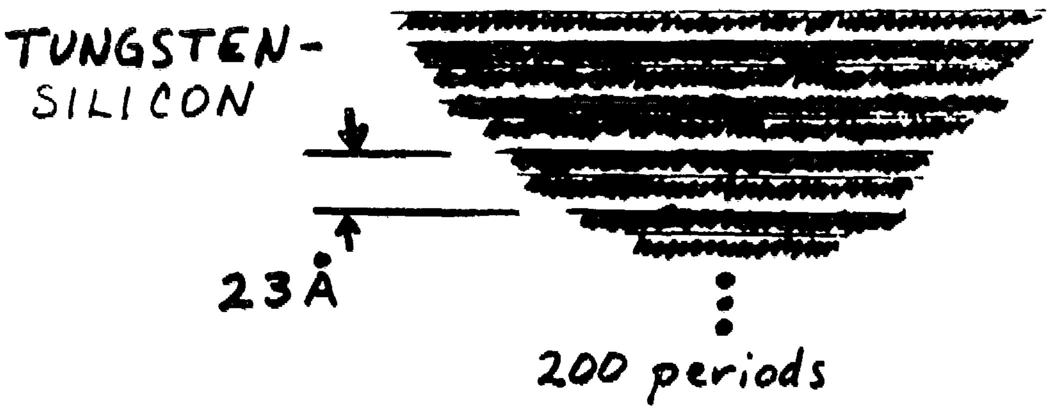
• Phase Separation in Al-Zn and Oxide Glass Systems

→ • Ordering in Cu_3Au

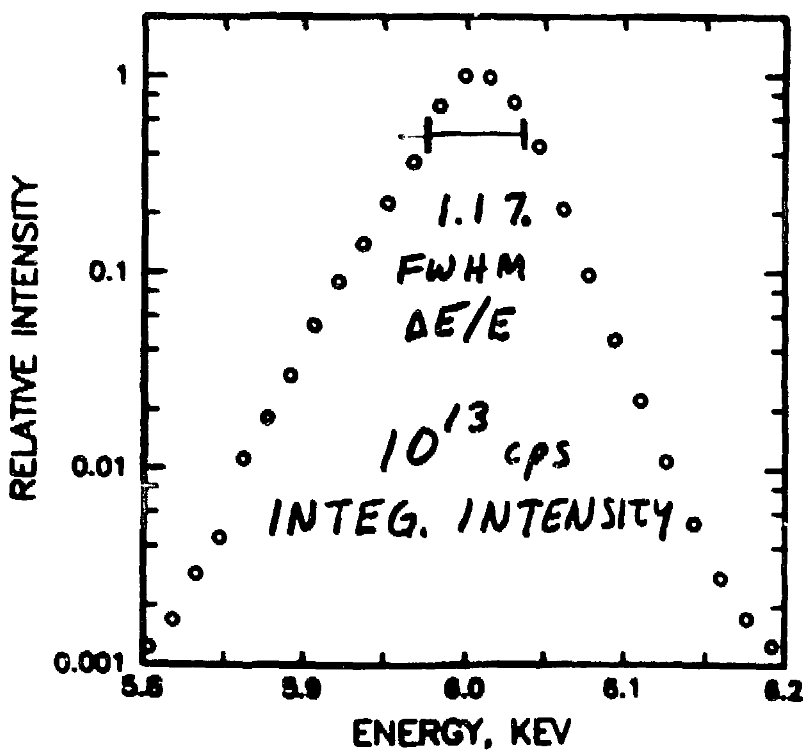
NSLS IBM/MIT BEAMLINES X-20A AND X-20C



WIDE-BANDPASS MONOCHROMATOR USING MULTILAYER OPTICS

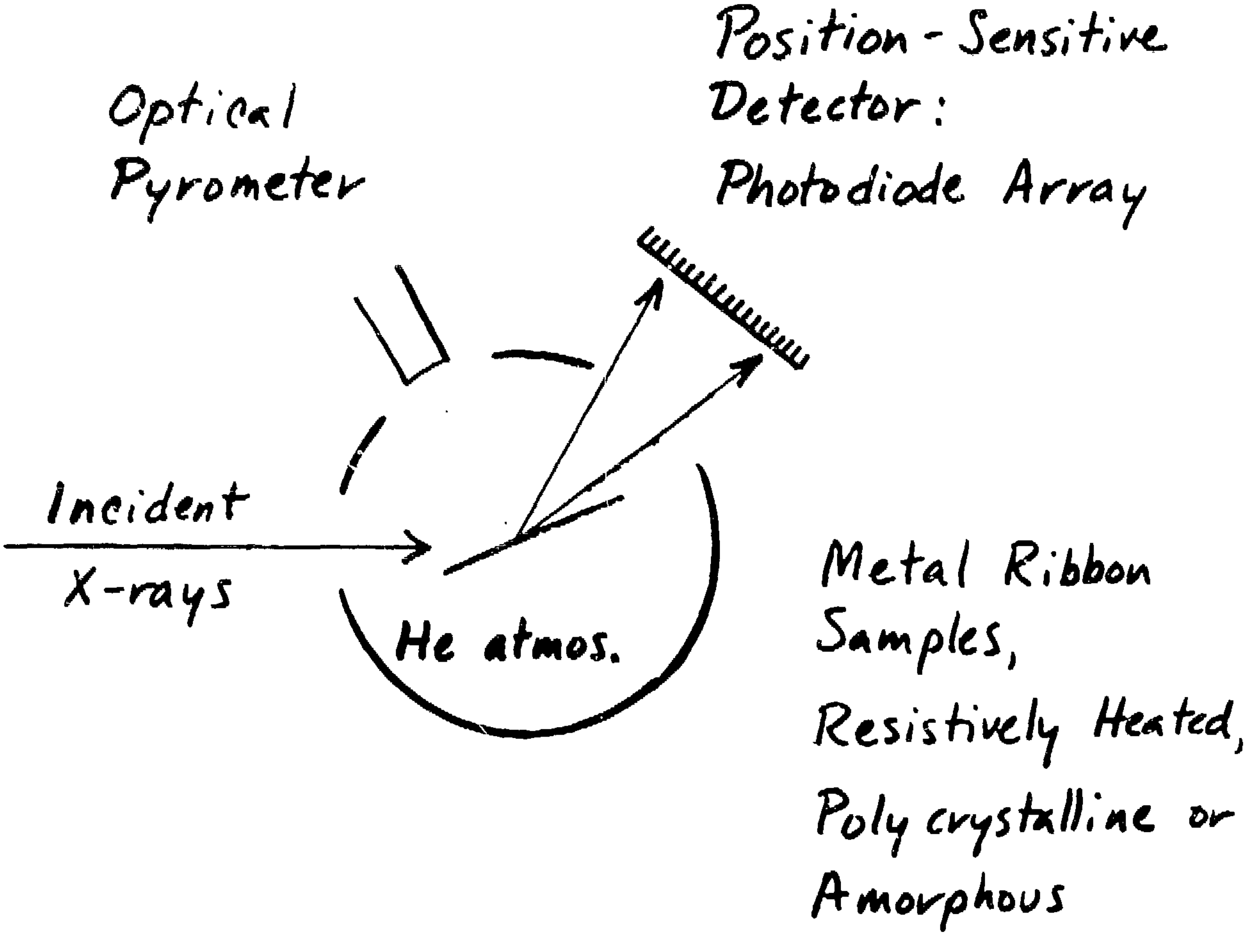


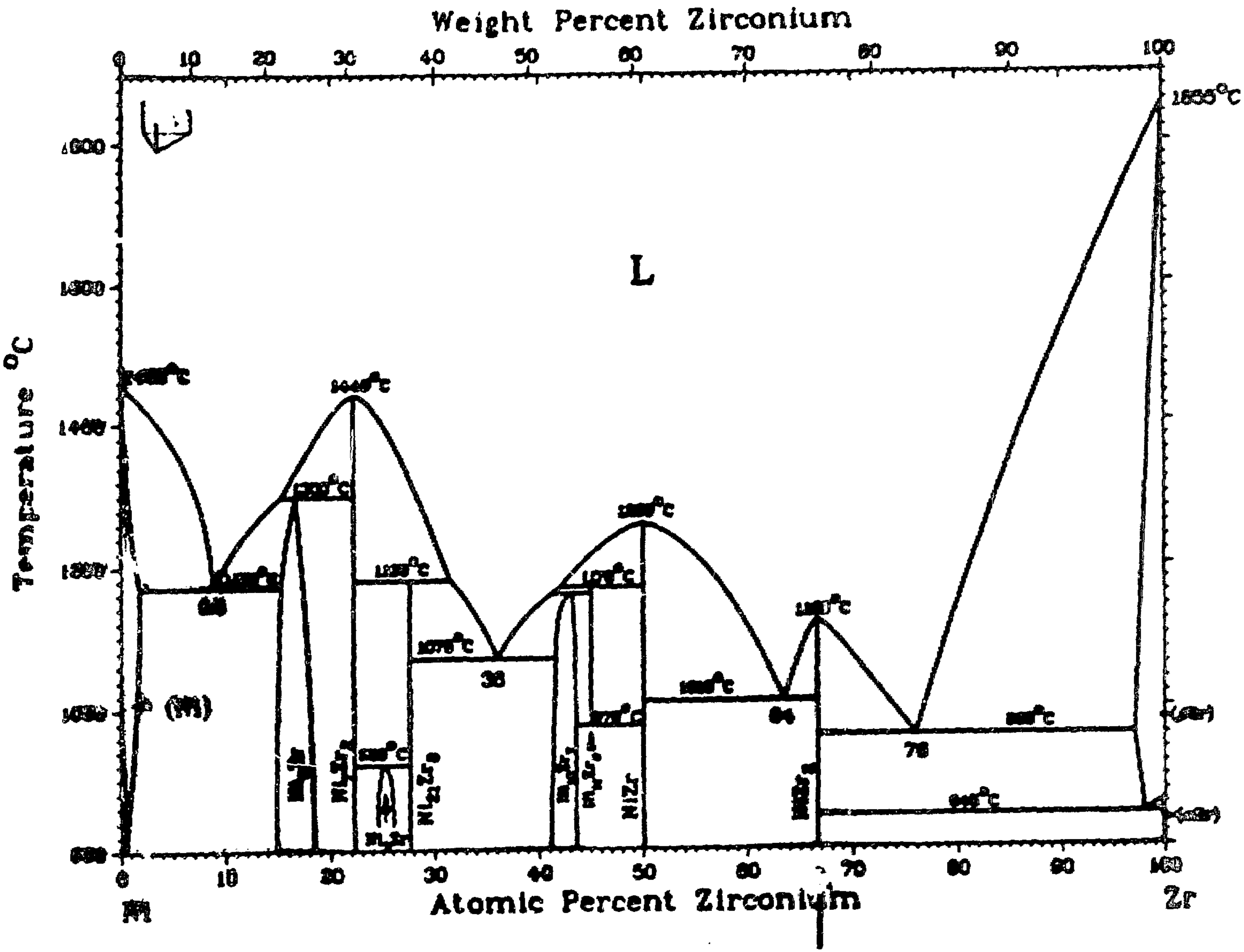
TYPICAL MONOCHROMATIC BEAM SPECTRUM:



MILLISECOND - RESOLUTION STUDIES OF PHASE TRANSITION KINETICS

EXPERIMENTAL GEOMETRY:





Weight Percent Zirconium
Atomic Percent Zirconium
Temperature °C
L
1855°C
Zr

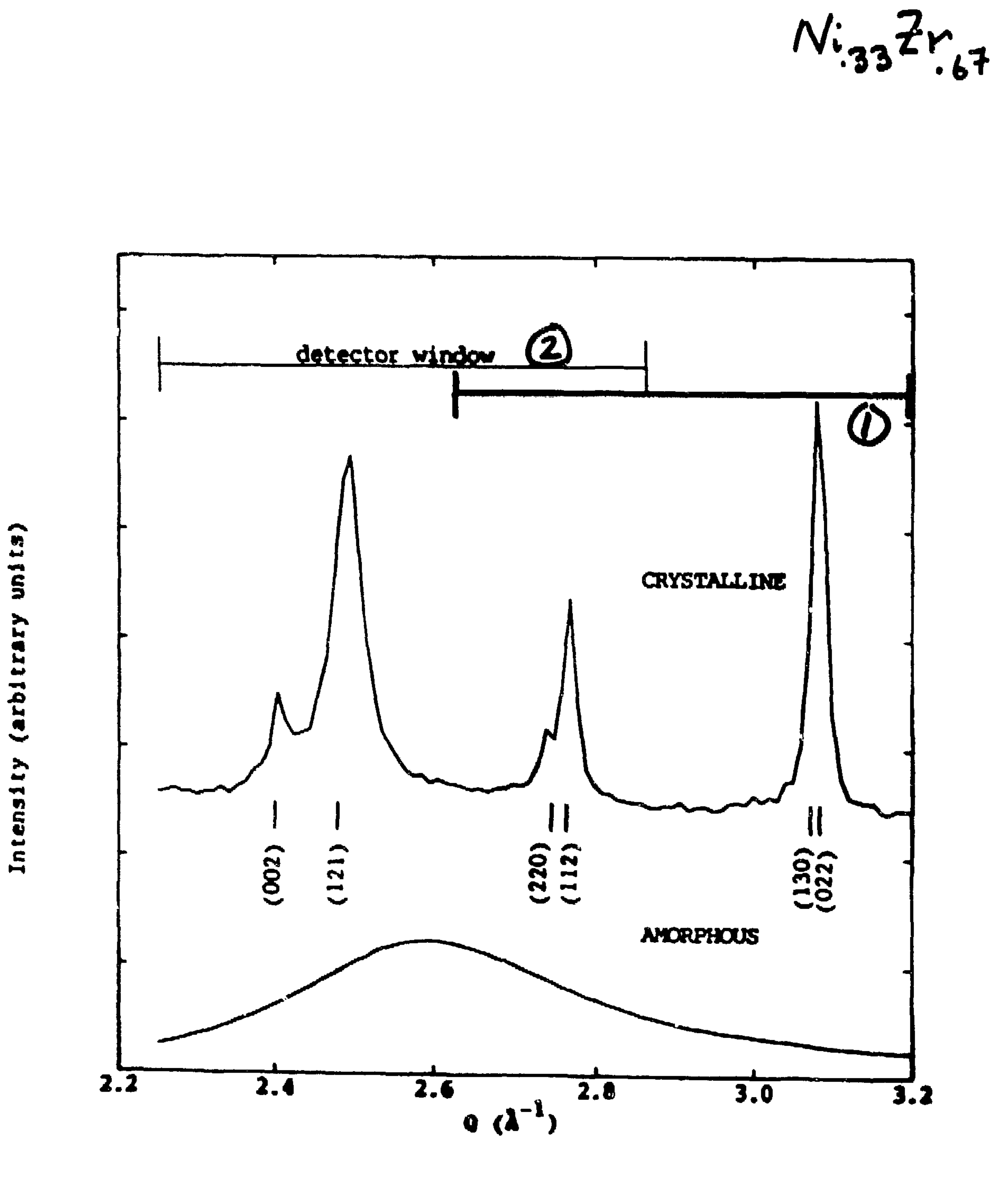
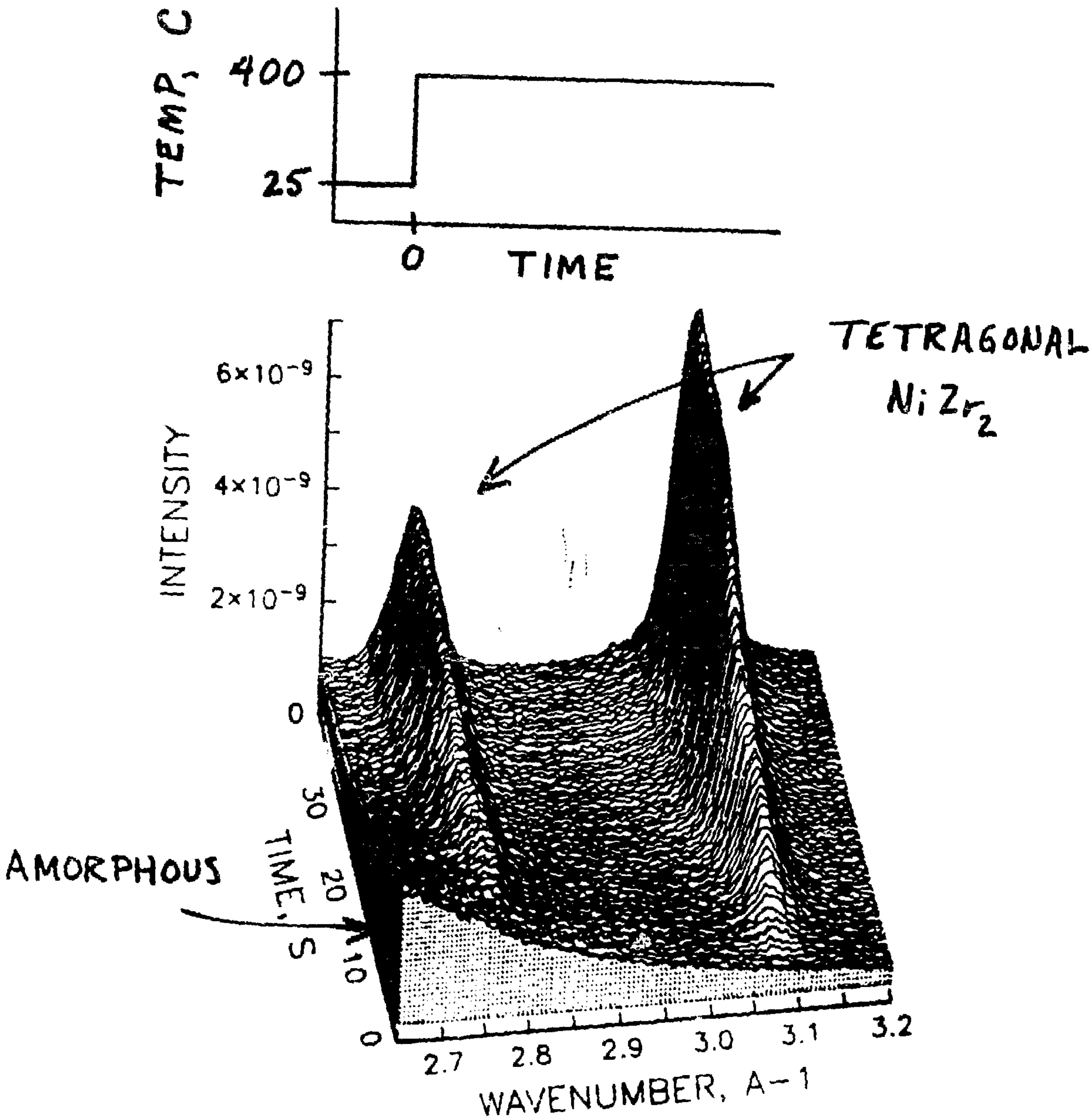

Ni.33Zr.67
detector window
2
1
CRYSTALLINE
AMORPHOUS
(002)
(121)
(220)
(112)
(130)
(022)
Intensity (arbitrary units)
2.2
2.4
2.6
2.8
3.0
3.2
Q (Å⁻¹)

Figure 1

CRYSTALLIZATION OF $Ni_{.33}Zr_{.67}$



B. STEPHENSON

Δt = 3 milliseconds per pattern

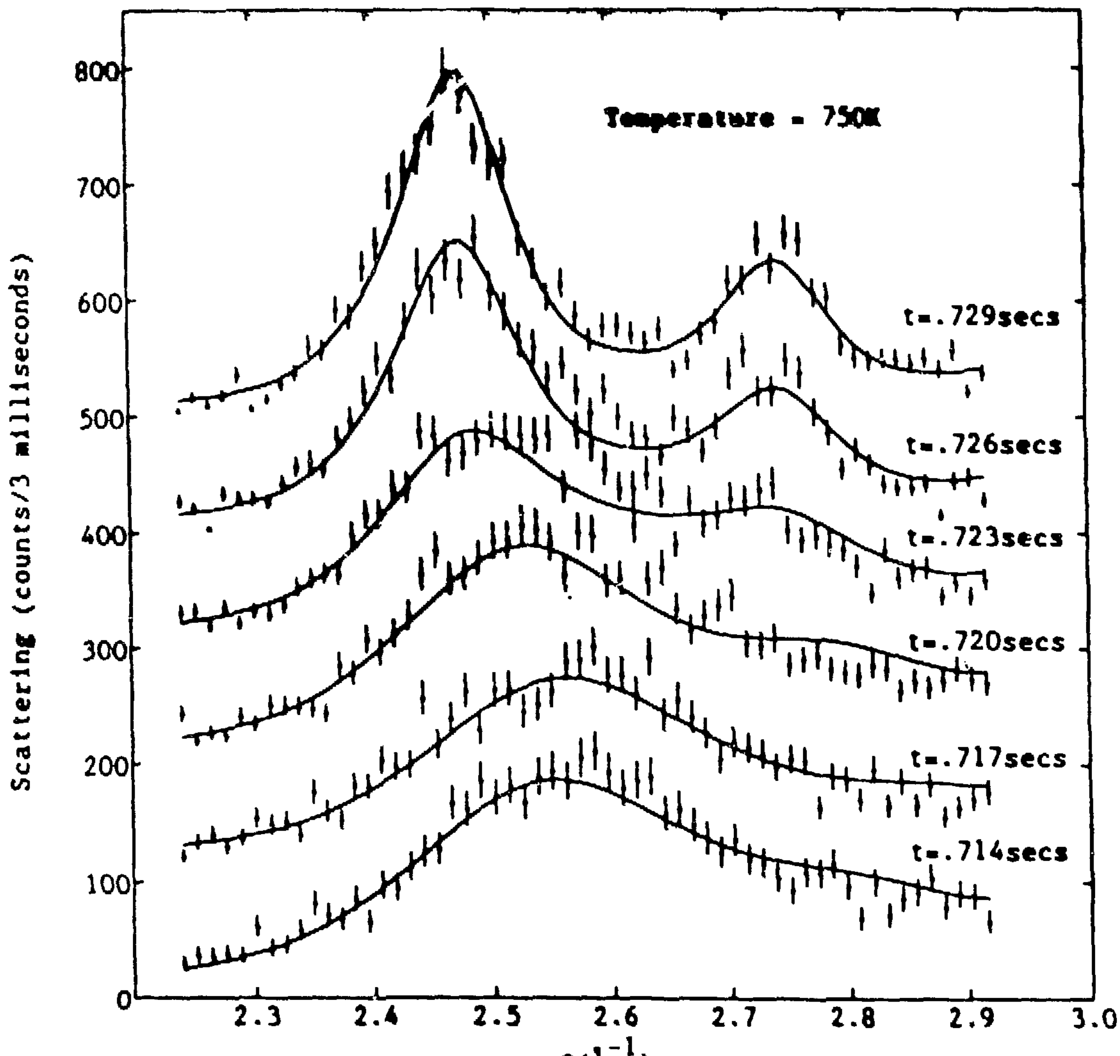
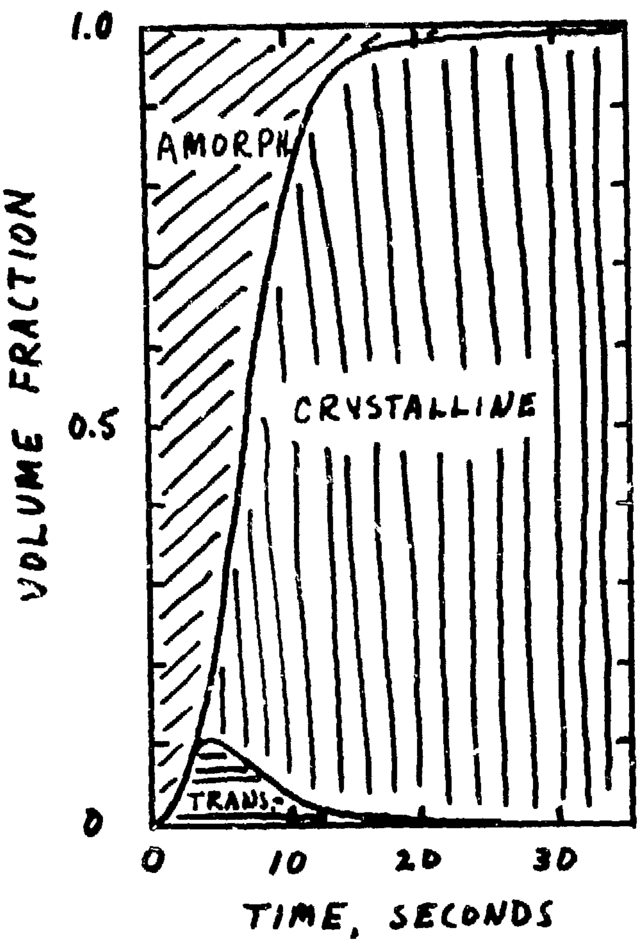
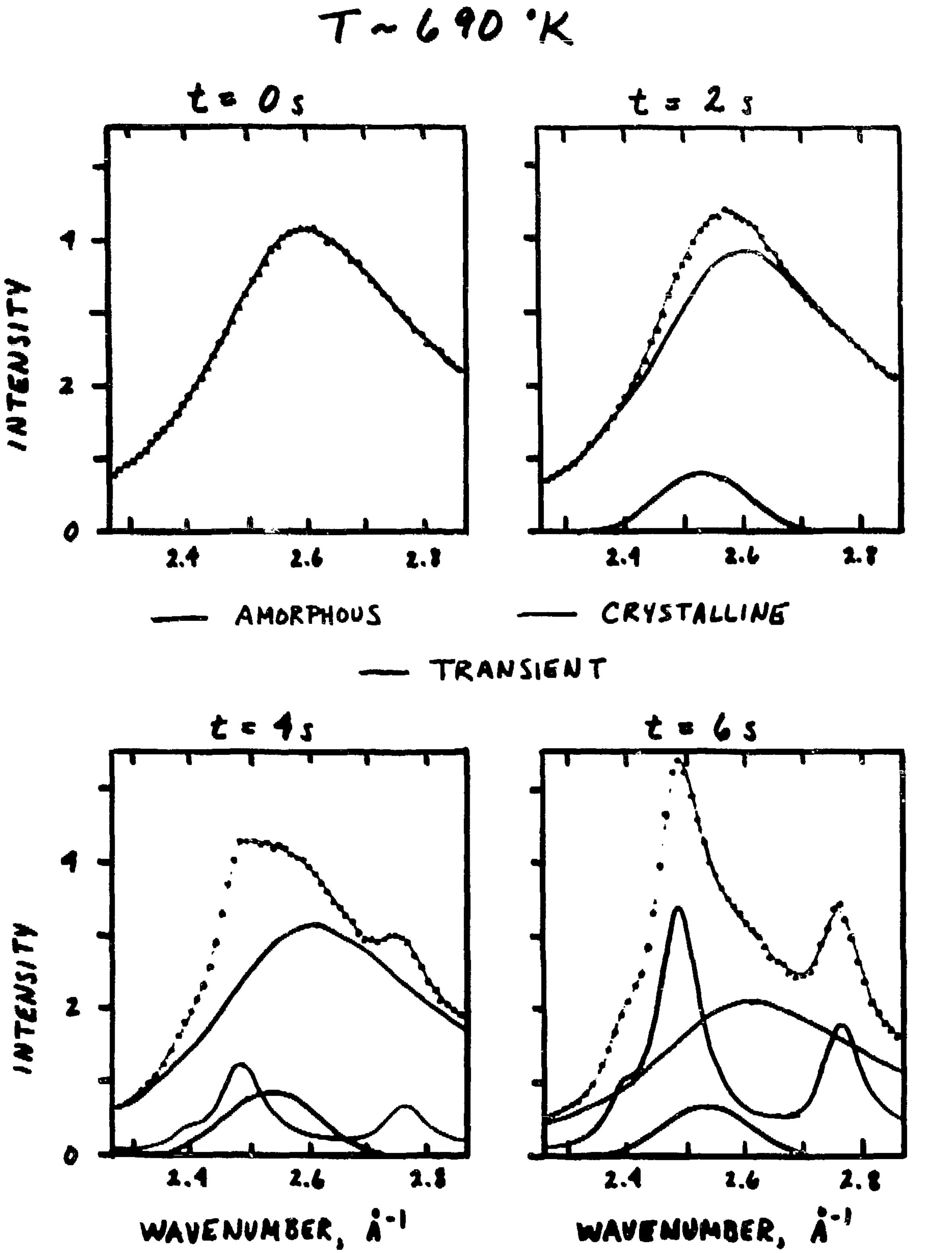
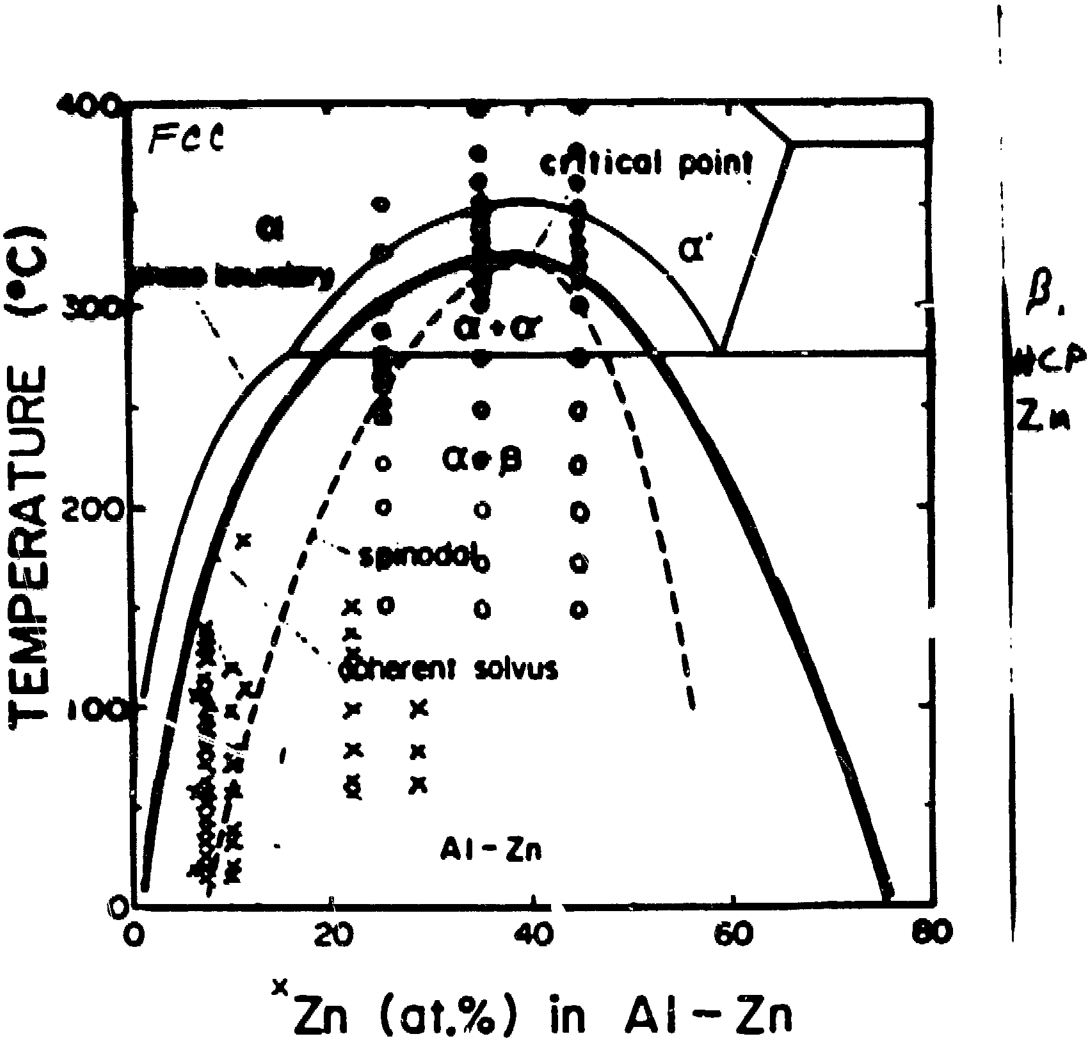


Figure 5

$$I(k,t) = [1 - x(t)]\, I_{AMORPHOUS}(k) + x(t)\,[1 - f(t)]\, I_{CRYSTAL.}(k) + x(t)\, f(t)\, I_{TRANSIENT}(k)$$



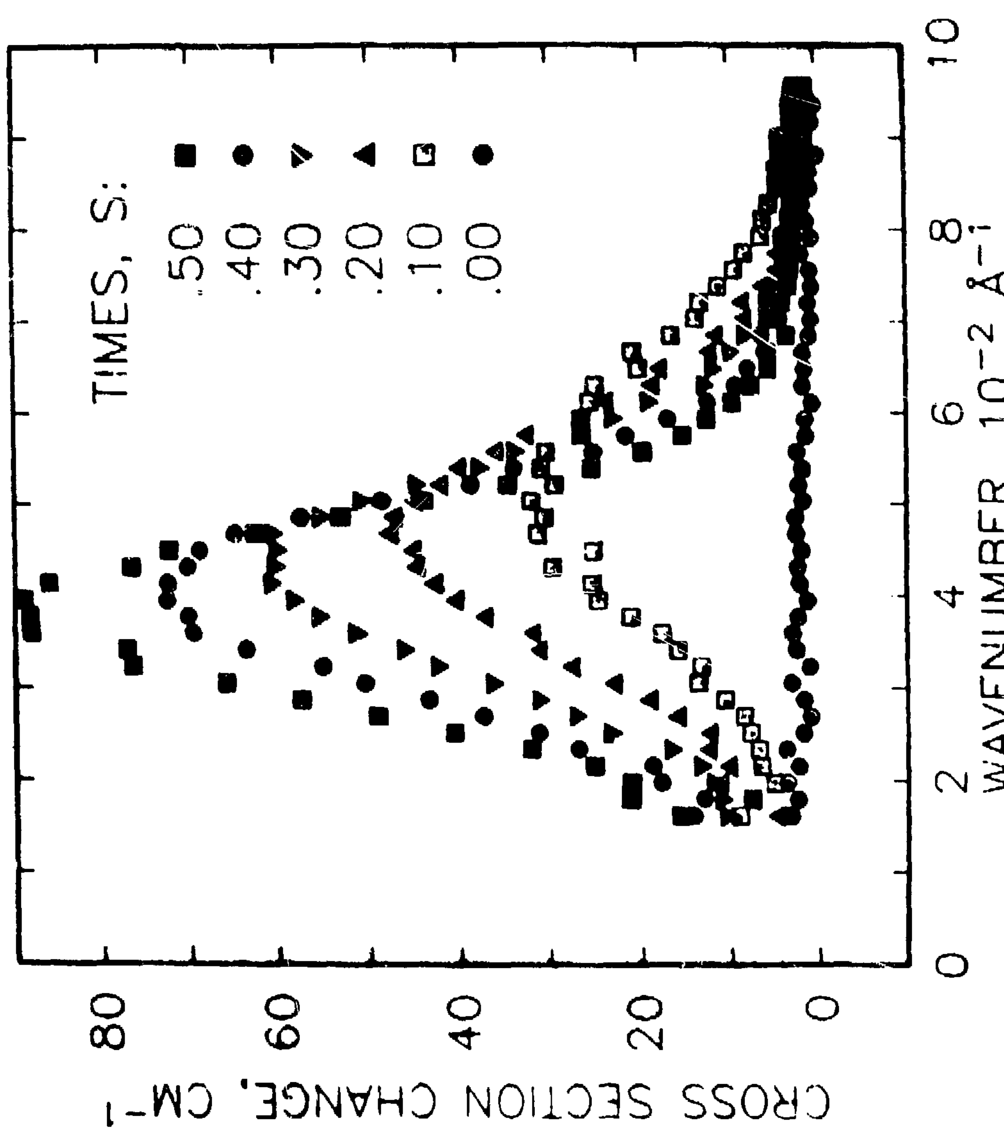

T ~ 690 °K
t = 0 s
t = 2 s
t = 4 s
t = 6 s
INTENSITY
0
2
4
2.4
2.6
2.8
AMORPHOUS
CRYSTALLINE
TRANSIENT
WAVENUMBER, Å⁻¹

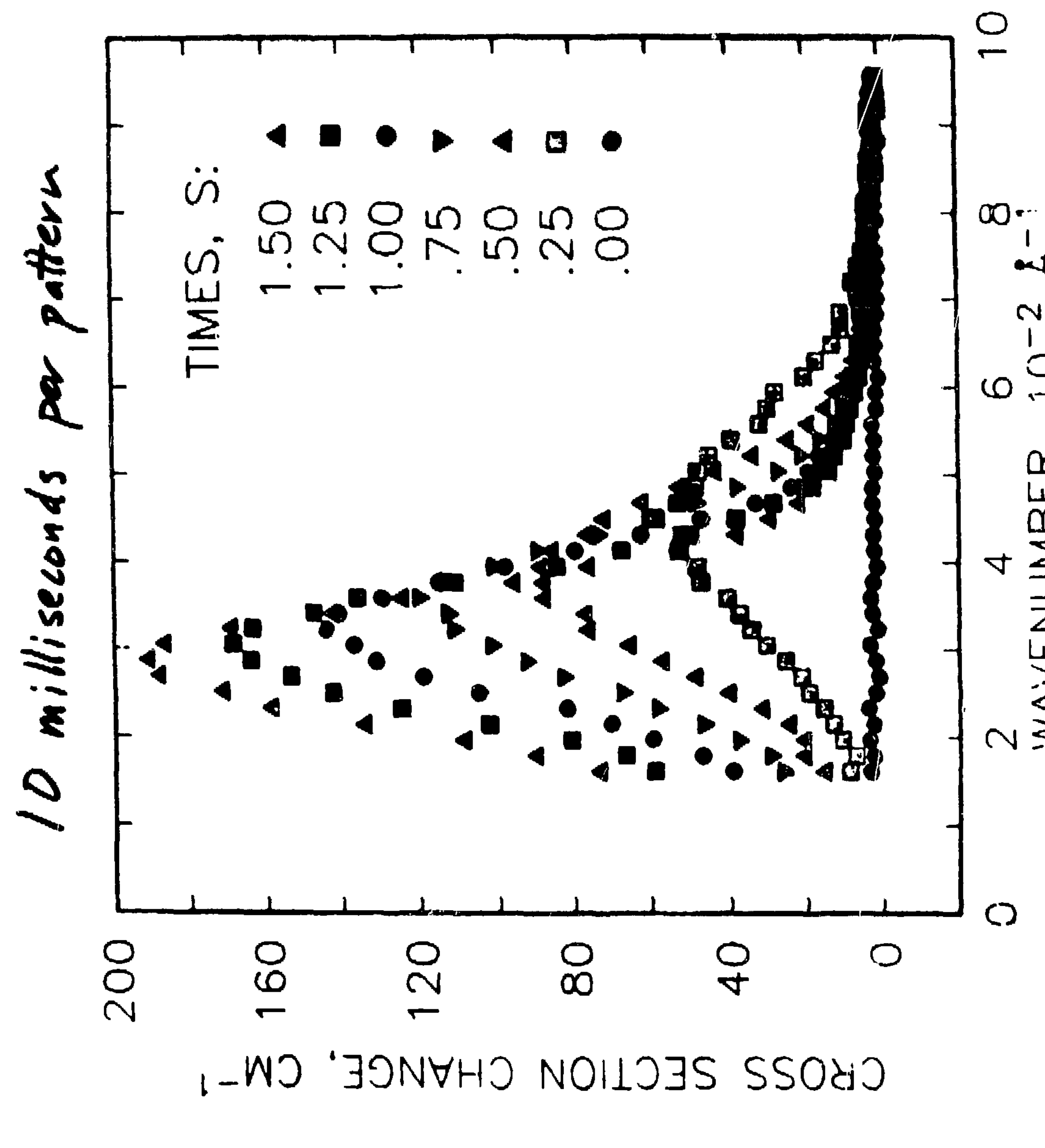


X - 12 previous studies,
1967 - 1985

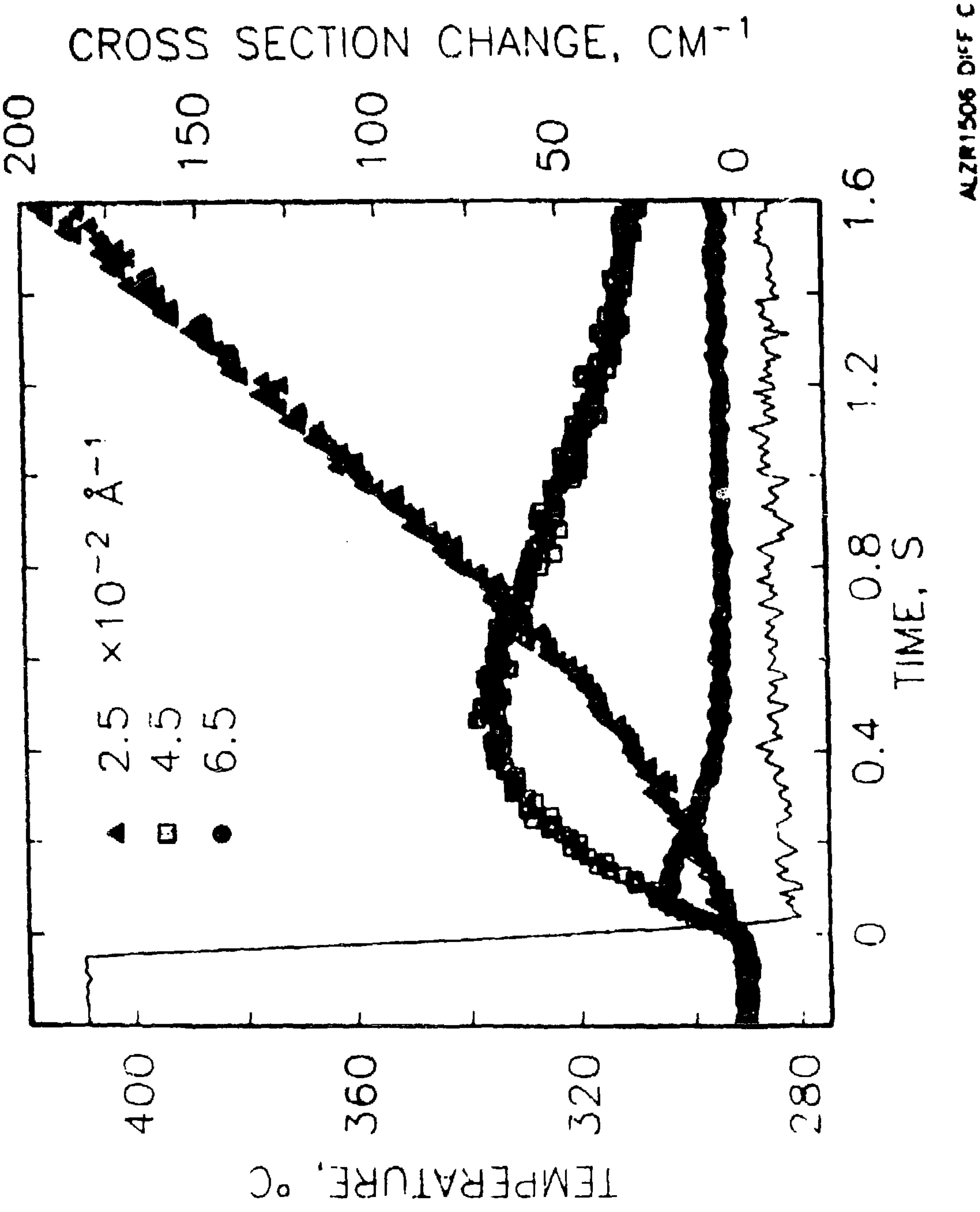
O - this work

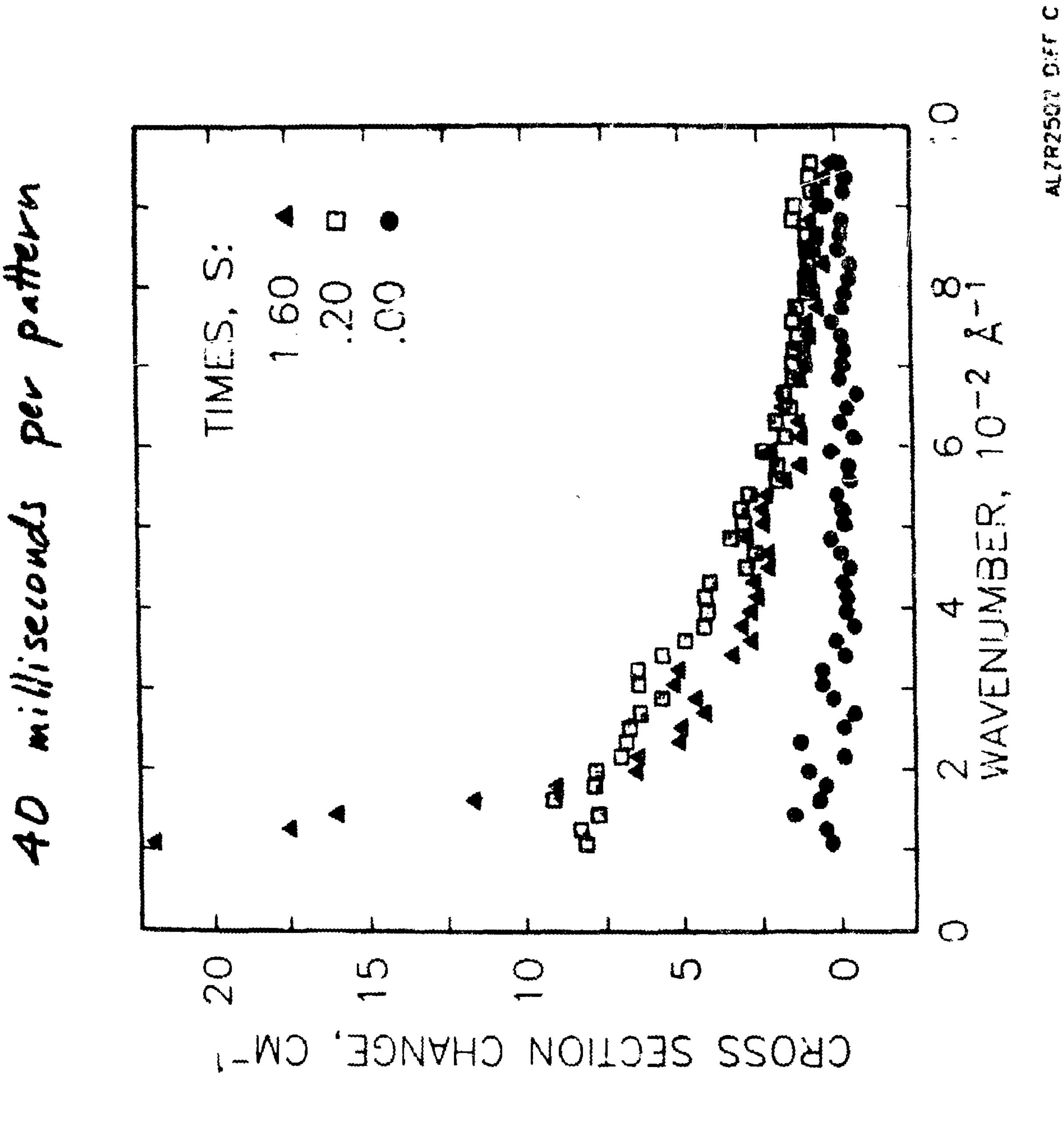
10 milliseconds per pattern



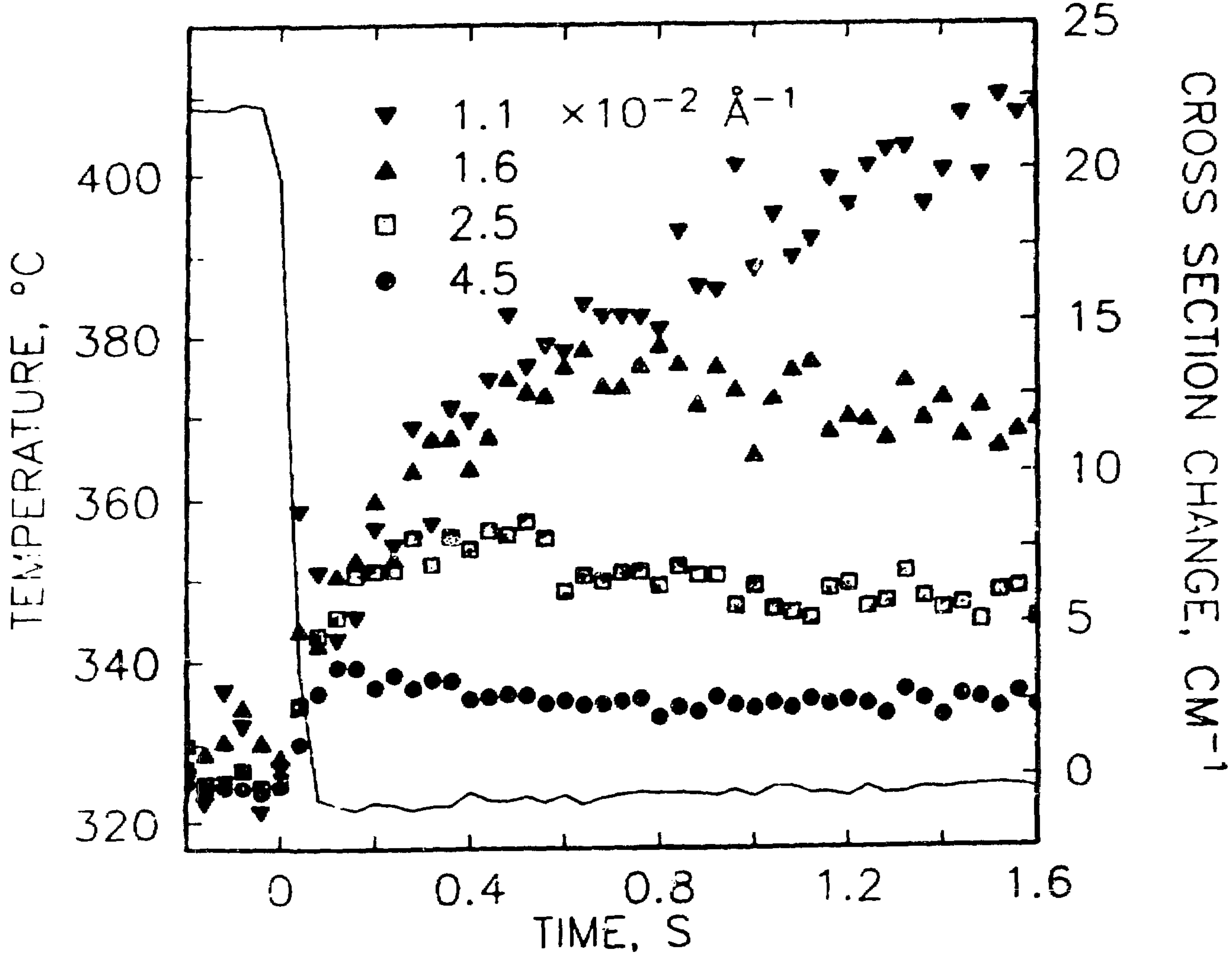


10 milliseconds per pattern
TIMES, S:
1.50
1.25
1.00
.75
.50
.25
.00
CROSS SECTION CHANGE, CM⁻¹
200
160
120
80
40
0
WAVENUMBER, 10^{-2} Å^{-1}
0
2
4
6
8
10


CROSS SECTION CHANGE, CM^{-1}
200
150
100
50
0
TEMPERATURE, °C
400
360
320
280
TIME, S
0
0.4
0.8
1.2
1.6
2.5 ×10^{-2} Å^{-1}
4.5
6.5
ALZR1506 DIFF C



40 milliseconds per pattern
TIMES, S:
1.60
.20
.00
WAVENUMBER, 10^-2 Å^-1
CROSS SECTION CHANGE, CM^-1
0
2
4
6
8
10
20
15
10
5
0



ALZR2502 DIFF C

SUMMARY

high-brightness source
multilayer monochromator
photodiode-array detector } ⇒

X-ray scattering patterns can be measured in milliseconds.

This allows in-situ studies of fast processes, e.g. kinetics of phase transitions.

New phenomena observed:

$NiZr_2$ - Transient structure during crystallization

Cu_3Au - Distinction between equilibration of SRO and nucleation

Al-Zn - Nonlinear early-stage spinodal decomposition near T_c

Time-Resolved Scattering Using a Position-Sensitive Detector

		NSLS Bend Mag.	APS Undulator
Low Resolution, $\Delta q/q \sim 10^{-2}$	Useful Intensity, cps	2×10^{13}	5×10^{15}
	Time per Pattern, sec	$10^{0} - 10^{-3}$	$10^{-3} - 10^{-6}$
High Resolution, $\Delta q/q \sim 2 \times 10^{-4}$	Useful Intensity, cps	$\sim 10^{10}$	10^{14}
	Time per Pattern, sec	$10^{3} - 10^{0}$	$10^{-1} - 10^{-4}$

SYNCHROTRON X-RAY MICROTOMOGRAPHY*

Keven L. D'Amico
Exxon Research and Engineering Co.
Annandale, New Jersey

ABSTRACT

We have developed a technique for viewing the internal, three-dimensional structure of small (1 mm) objects with a spatial resolution of approximately 10 microns. The technique is referred to as "microtomography" and is based on the same physical principles as are conventional medical CAT and NMR tomography procedures. Our technique employs synchrotron radiation as the x-ray probe. We have used the system for a series of preliminary experiments at the Brookhaven NSLS, where we are currently building a dedicated beam line for tomography studies. The unique features and intensity of the synchrotron beam make a wide variety of studies possible. The technique promises to have application to many areas of materials science and medicine. We will describe the principles of the technique and show the apparatus required for taking tomography data. Representative data will be shown that illustrate the capabilities of the technique.

Reference

B.P. Flannery, H.W. Deckman, W.G. Roberge, and K.L. D'Amico, Science 237:1439 (1987).

*The following abstract and copies of viewgraphs were provided by the speaker.

TOMOGRAPHY EFFORT
COLLEAGUES AT EXXON

• H.W. DECKMAN J.M. DUNSMUIR S.M. GRUNER	DETECTOR DEVELOPMENT
• B.P. FLANNERY W.G. ROBERGE M.S. WAINGER	RECONSTRUCTION ALGORITHMS
• R.C. HEWITT M. SANSONE	BEAMLINE DEVELOPMENT

P. EISENBERGER

NATIONAL SYNCHROTRON LIGHT SOURCE
BROOKHAVEN NATIONAL LABORATORY
UPTON, NY

(SUPPORTED BY US DOE #DEAC0276CH00016)

OUTLINE

- GENERAL INTRODUCTION
  - –MEDICAL TOMOGRAPHY
  - –MICROTOMOGRAPHY
  - –SYNCHROTRON RADIATION
- TOMOGRAPHIC TECHNIQUES
  - –GENERAL CONCEPTS
  - –NUMERICAL DATA ANALYSIS
  - –INSTRUMENTATION
- MICROTOMOGRAPHY
  - –MOTIVATION
  - –TECHNICAL CHALLENGES
  - –DATA ACQUISITION
- RESULTS
  - –STANDARD SAMPLES
  - –UNKNOWNS
  - –QUANTITATIVE RESULTS
- FUTURE DIRECTIONS
  - –DETECTOR SYSTEM
  - –DEDICATED BEAMLINE
  - –SCIENTIFIC ISSUES

OUTLINE

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  - –MEDICAL TOMOGRAPHY
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  - –STANDARD SAMPLES
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  - –QUANTITATIVE RESULTS
- FUTURE DIRECTIONS
  - –DEDICATED BEAMLINE
  - –SCIENTIFIC ISSUES

GENERAL INTRODUCTION

WHAT IS TOMOGRAPHY?

- –TECHNIQUE FOR DETERMINING THE INTERNAL STRUCTURE OF AN OBJECT
- –BASED ON MEASUREMENT OF THE INTERACTION OF A PROBE BEAM WITH THE MATERIAL
- –MEDICAL X–RAY TOMOGRAPHY DEVELOPED BY HOUNSEFIELD AND CORMACK
- –NMR TOMOGRAPHY DEVELOPED BY LAUTERBUR

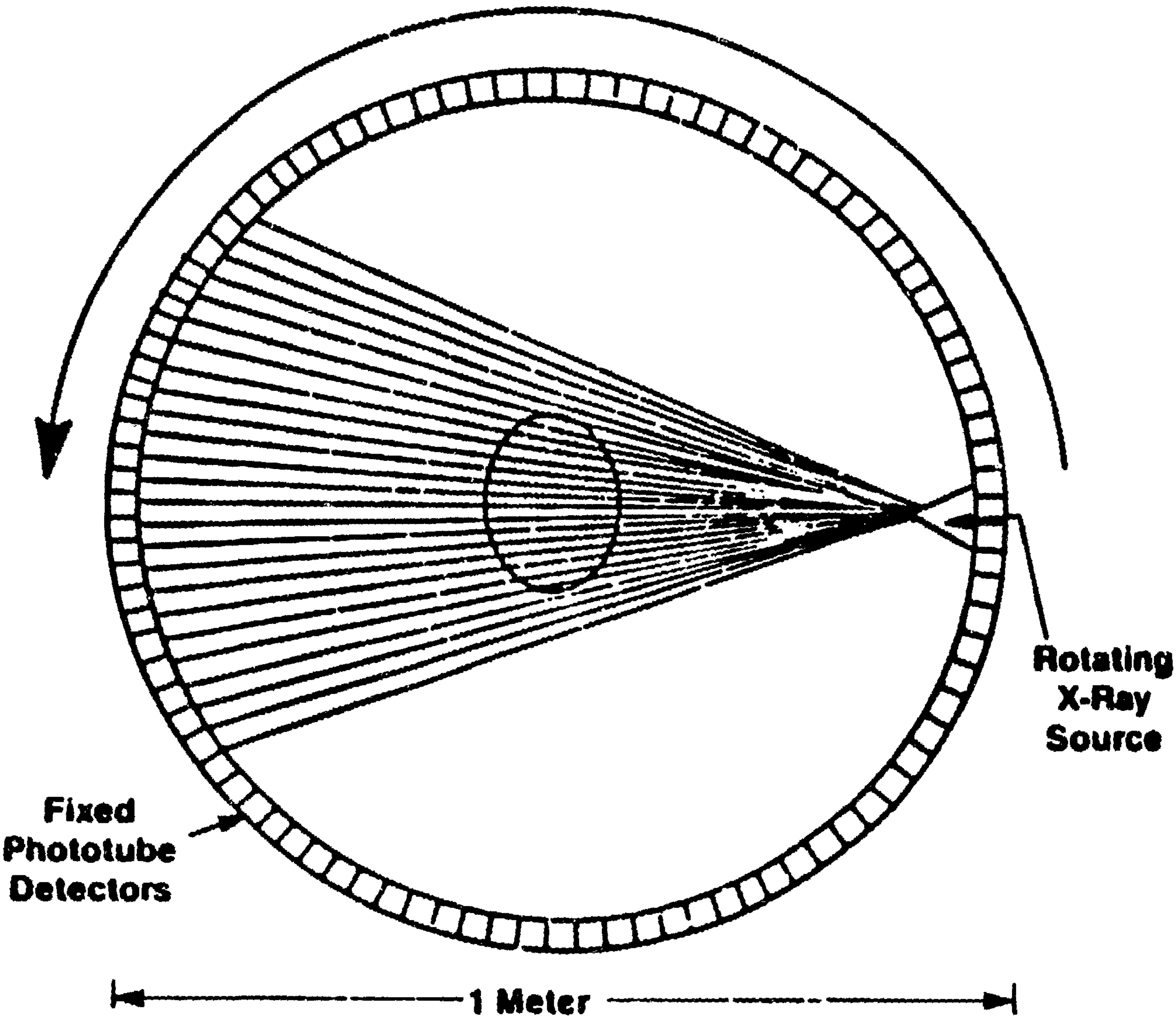
•BOTH TECHNIQUES WIDELY USED FOR MEDICINE

•X–RAY TECHNIQUE ALSO WIDELY APPLIED TO NON–DESTRUCTIVE EVALUATION

- –CORE FLOODS
- –SOLID ROCKET MOTORS
- –TURBINE BLADES
- –CERAMICS

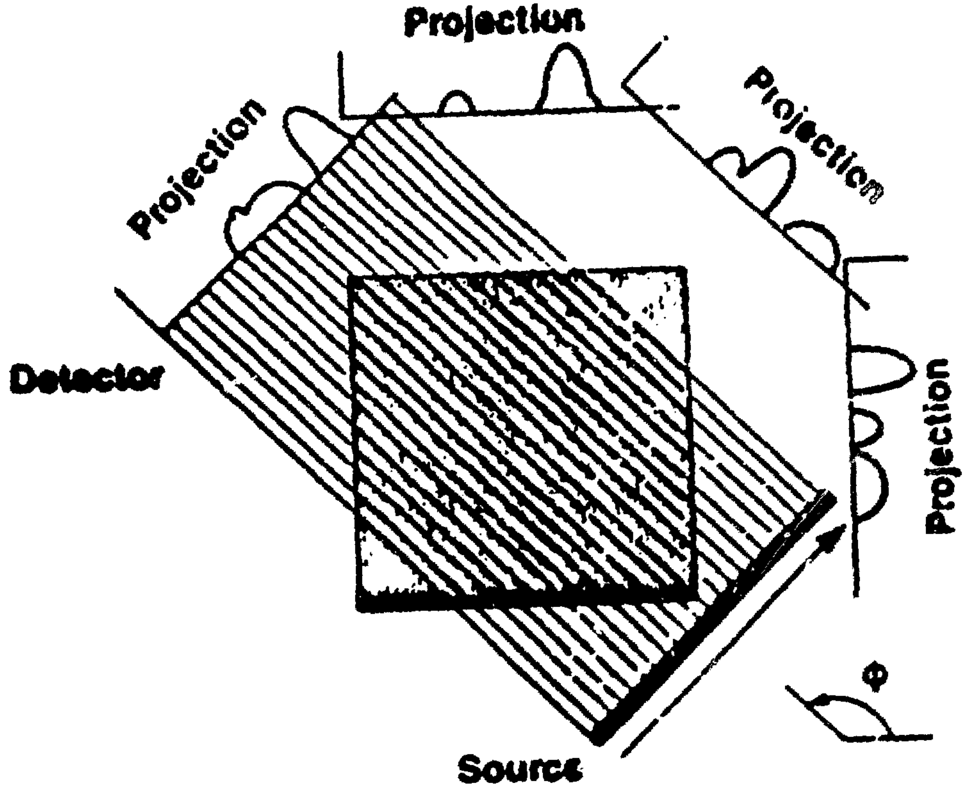
CONVENTIONAL MEDICAL CAT SCANNER

- 1 MM RESOLUTION
- 256 X 256 PLANAR IMAGE



TOMOGRAPHIC DATA ACQUISITION

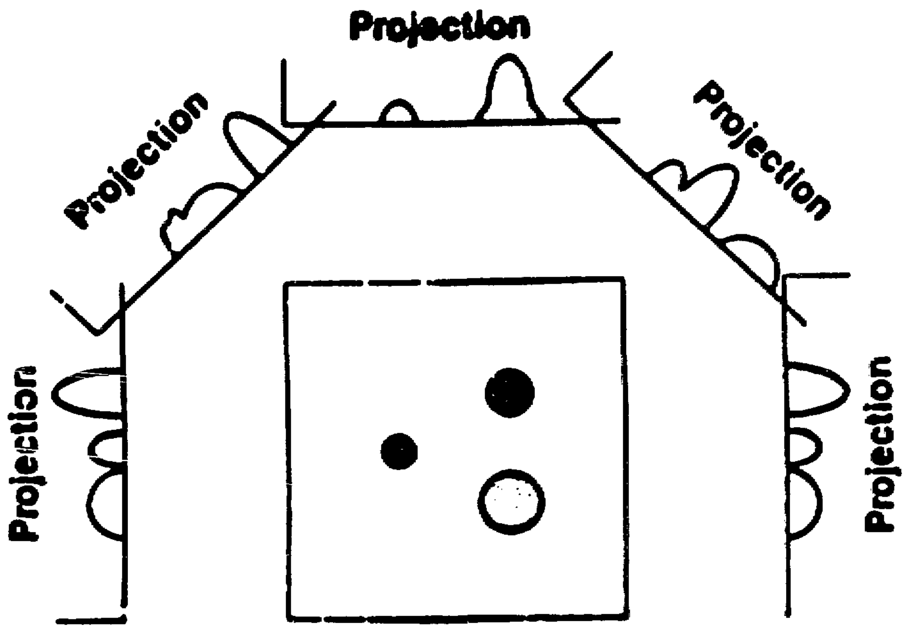
PLANE PARALLEL X–RAYS: SCHEMATIC



- DETECTOR MEASURES TRANSMITTED INTENSITY ALONG COPLANAR RAYS OF BEAM FOR MANY VIEW ANGLES
- PROJECTION= ln(CALIBRATION/TRANSMITTED)

TOMOGRAPHIC DATA INVERSION

RESULT



•INVERSION RECOMBINES THE PROJECTION DATA TO DETERMINE ATTENUATION COEFFICIENT IN THE OBSERVED PLANE OF THE SAMPLE

GENERAL INTRODUCTION

MICROTOMOGRAPHY

- THE EXTENSION OF TOMOGRAPHY TECHNIQUES TO SMALLER MATERIALS AND HIGHER RESOLUTION
- NO FUNDAMENTAL REASON WHY THIS SHOULDN'T WORK
- IN PRACTICE THERE ARE TECHNICAL PROBLEMS
- FOR THE CASE OF X-RAY TOMOGRAPHY
  - DETECTORS WITH SUFFICIENT SPATIAL RESOLUTION
  - X-RAY SOURCE WITH SUFFICIENT FLUX
  - MECHANICALLY STABLE SAMPLE MOUNTS
  - MATHEMATICS AND STATISTICS OF PROCESS

MICROTOMOGRAPHY PROJECT

TOMOGRAPHY: A NON–DESTRUCTIVE IMAGING TECHNIQUE BASED ON ATTENUATION OF PENETRATING RADIATION

- GOAL: USE SYNCHROTRON X–RAY SOURCE TO CREATE IMAGES WITH MICRON RESOLUTION AND 1% PRECISION IN THE DETERMINATION OF THE DENSITY (ATTENUATION COEFFICIENT)

- FEATURES:
  - –RESOLUTION 1000 TIMES BETTER THAN MEDICAL CAT SCANNER
  - –COMPLETE 3D MAPS OF INTERNAL STRUCTURE
  - –SMALLER SAMPLE SIZE

- PRINCIPAL INNOVATIONS:
  - –HIGH RESOLUTION DETECTOR
  - –FAST METHODS FOR DATA INVERSION
  - –SYNCHROTRON X–RAY SOURCE

NOVEL PROBE FOR HETEROGENEOUS MATERIALS

See Nuclear Instruments and Methods B206(3): 542 (1983) proposal No 86-005

DEVELOPMENT OF COMPUTED TOMOGRAPHIC IMAGING SYSTEM USING MONOCHROMATIC X-RAYS

Katsuhisa USAMI, Koozoo SAKAMOTO, Hiroshi KOZAKA, Tatsumi HIRANO,
Yoshio SUZUKI[*], Kazunobu HAYAKAWA[*], Hidemi SHIONO[**] and Hideki KOONO[**]
Hitachi Research Lab., Hitachi Ltd., Hitachi Ibaraki
* Advanced Research Lab., Hitachi Ltd., Kokubunji Tokyo
** Central Research Lab., Hitachi Ltd., Kokubunji Tokyo

Introduction

X-ray computed tomography (CT) is a method for reconstructing the distribution of linear absorption coefficients in the cross section of a sample. This technique seems to be an attractive method for non-destructive evaluation of industrial materials. However, it is necessary to improve the performance factors of CT scanners such as contrast sensitivity, accuracy of attenuation coefficients, and space resolution. The use of a tunable and monochromatic X-ray source is one advantageous method for these purposes.

A CT scanner with a monochromatic X-ray source using synchrotron radiation was developed and trial CT images were obtained for several samples as reported herein.

Instrument

Fig.1 shows a schematic of the developed monochromatic X-ray CT scanner. Synchrotron radiation is monochromatized by a channel-cut momochromator. The beam size is 30 mm wide and 0.1-1 mm high. Two channel-cut monochromator, Si(220) and Si(400), are utilized. A set of transmitted X-ray intensities is measured by rotating the sample. A 1024 channel array detector, 25 μm wide x 2.5 mm high, which is a photodiode array with a scintillator, is used.

In this system, space resolution is determined by the detector resolution. Modulation transfer function (MTF) measurements indicate the resolution is 0.12 mm. A feature of this system is that the projection image can be magnified by an asymmetrical Bragg reflection. Resolution of 0.03 mm is attained by a five-fold magnification.

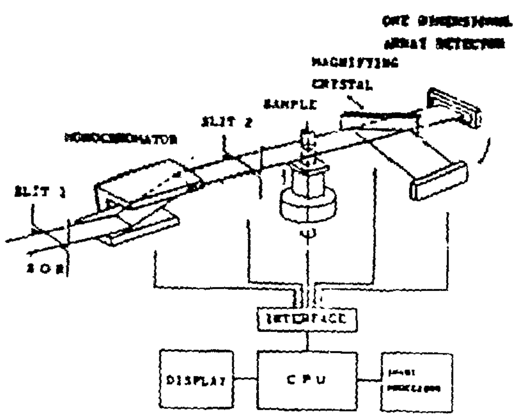


Fig.1 Schematic layout of the computed tomographic imaging system using monochromatic X-rays.

Results

Tests of the scanner were carried out and trial CT images were obtained. Fig.2 shows the CT image of an okra cross section. Complex and fine structures such as the thin membranes between the seeds are clearly oberved.

The advantage of using a monochromatic X-ray source is that the diatibution of an alement of a cross section can be obtained by the difference between CT images at higher and lower energies than the absorption edge energy. Fig.4 shows test results for an elemental distribution. The Mo image is exructed by the difference of the CT images (A) and (B)

References

1) Yu.I.Borodin et al., Nucl. Instr. and Meth. A246 (1986) 649.
2) A.C.Thompson et al., Nucl. Instr. and Meth. 222 (1984) 319.

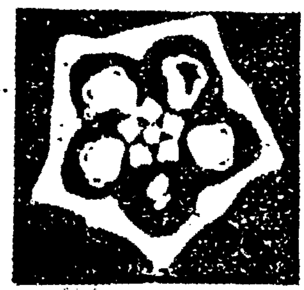
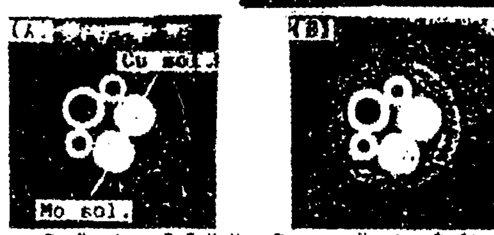


Fig.2 CT image of okra.
Energy = 15 KeV.
Slice width = 0.3 mm.



E = Mo K-edge+0.6 KeV E = Mo K-edge-0.4KeV.

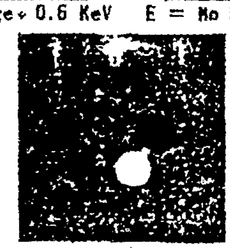
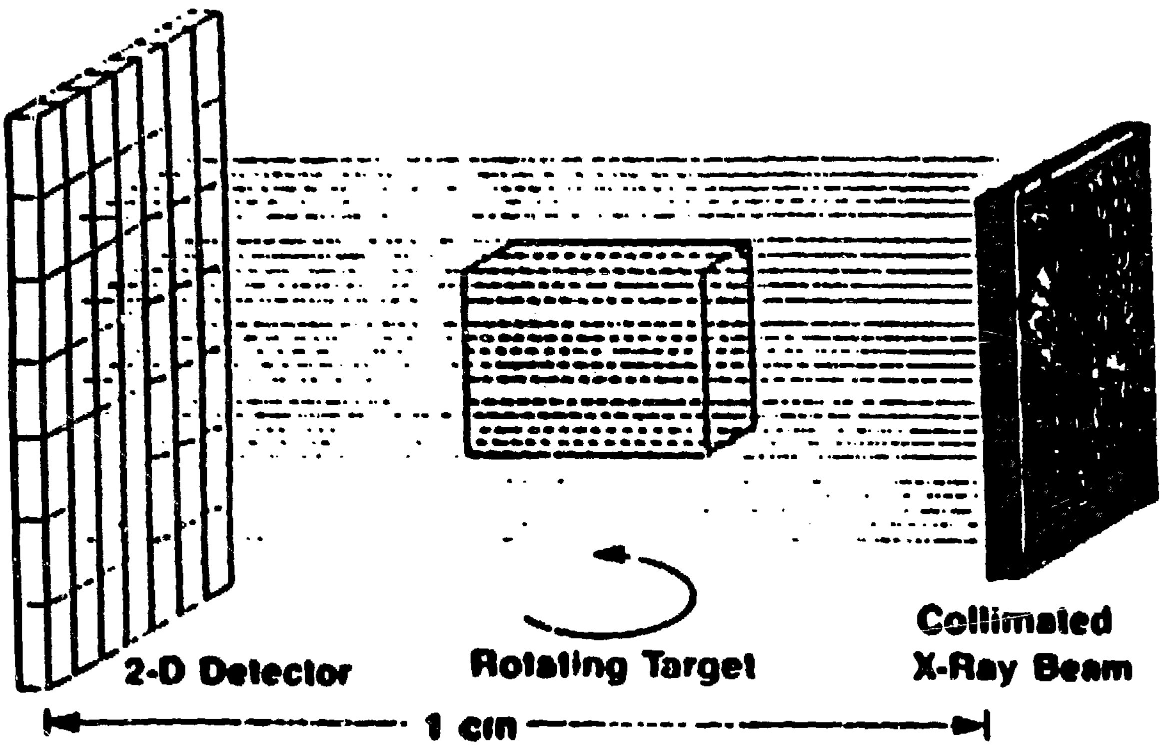


Fig.3 Mo image obtained by the difference of CT images (A) and (B).

EXXON 3D
MICROTOMOGRAPHY SYSTEM

- •1 MICRON RESOLUTION
- •500 X 500 PLANAR IMAGE
- •3D DATA SET: 300 PLANES



The energy of the incident x-ray beam can be selected using a single-crystal monochromator, but most synchrotron beam lines use a double-crystal configuration to restore the x-ray beam to its original direction. The double-crystal arrangement also helps remove higher-order harmonics that also satisfy the Bragg conditions. The energy resolution is typically in the range from 0.1 to 0.01% over energies ranging from 4 to 70 keV, and higher energy resolution can be obtained by using dispersively oriented crystals.

The rotating sample stage enables us to use computed tomography (CT) reconstruction algorithms to obtain true three-dimensional images of chemical distributions within the sample. The spatial resolution after magnification, determined by the quality of the phosphor coatings, is 4 to 5 μm in three dimensions.

Why Synchrotron Radiation?

Three x-ray source parameters—x-ray intensity, energy spectrum, and divergence of the incident beam—determine the spatial resolution and sensitivity of our camera. The intensity of the radiation source determines the exposure time to achieve a given signal-to-noise ratio. In two-dimensional imaging, this ratio scales with the square root of the exposure (increasing the exposure 100-fold decreases the uncertainty in the x-ray data by a factor of 10). Because of the way errors propagate in the reconstruction algorithms of three-dimensional CT, determining the signal-to-noise ratio depends on the sensitivity and spatial resolution desired. Here, sensitivity is considered to be the ability to recognize small changes in absorption, above the background noise, between adjacent pixels. A sensitivity of 1% means that changes in sample contrasts of 1% can be measured. The fluence required for a given sensitivity is inversely proportional to sensitivity; a sensitivity of 10% requires 100 times less fluence than a sensitivity of 1%.

Figure 2 gives the relationship between resolving power and required fluence (conservatively estimated) to achieve a sensitivity of 1% in CT. (The resolving power is given by the ratio of the maximum sample diameter to the width of a pixel; imaging a 1-mm sample to 1-μm resolution requires a resolving power

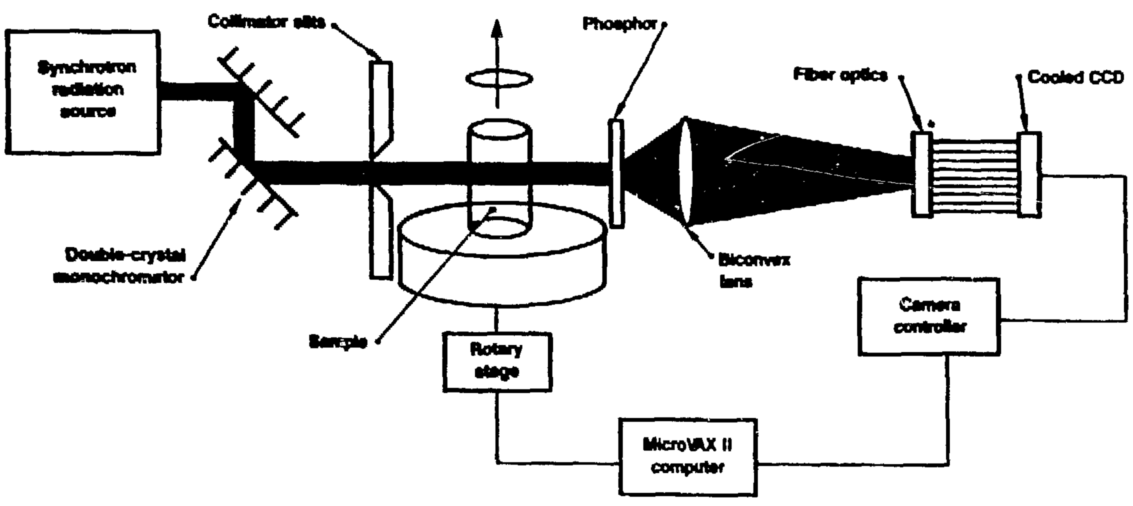
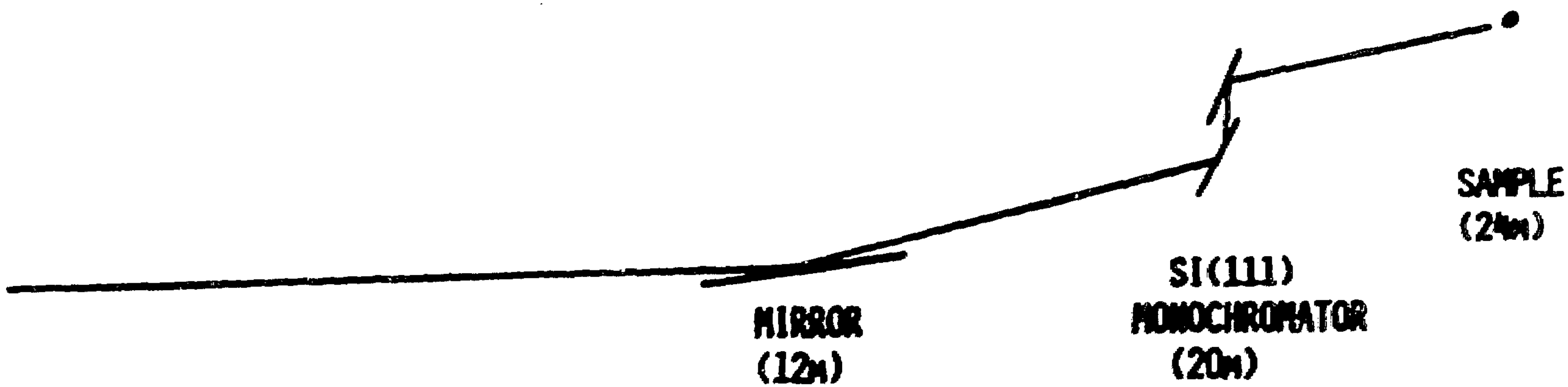


Figure 1. The experimental assembly for performing high-resolution x-ray imaging. After they pass through the sample, x rays are converted into visible light in a phosphor that is focused on a fiber-optic image plane by a biconvex lens. The optical fibers transmit the image to the CCD, from which it is read out in digital form by the camera controller and routed to the computer. The specimen can be held motionless for two-dimensional imaging (dichromography) or topography, or rotated to obtain the multiple images needed for computed tomography.

X10A BEAMLINE SCHEMATIC



- FEATURES
  - COMPUTER CONTROLLED/STEPPING MOTOR DRIVEN
  - 10(E11) PHOTONS/S FOCUSSED MONOCHROMATIC BEAM
  - FLEXIBLE CONFIGURATIONS
- BEAMLINE STAFF
  - RICH HEWITT
  - MIKE SANSONE, STEVE CONSTANTINO, BILL VARADY
  - RANDY ABROMAWITZ, STEVE BENNETT, BOB WIESER
  - GARY NINTZEL

SUMMARY

HIGHLIGHT IMPORTANT FEATURES

- RESOLUTION
  - CURRENTLY <10 MICRONS
  - APPROACHING 1 MICRON
  - VARIABLE 1–50 MICRONS

- SAMPLES
  - WIDE VARIETY POSSIBLE
  - MANY CUSTOM CELLS POSSIBLE

- SENSITIVITY
  - 5% DIFFERENCES IN ABSORPTION COEFFICIENT
  - CHEMICAL ANALYSIS THROUGH ABSORPTION EDGE
  - FIRST ROW TRANSITION METALS IDEAL

- DATA SET
  - FULL THREE DIMENSIONAL INFORMATION ACQUIRED
  - QUANTITATIVE ANALYSIS POSSIBLE

SUMMARY

IMPACT OF NEXT GENERATION SOURCE

- MOST IMPORTANT FEATURES OF SOURCE
  - –INTRINSIC COLLIMATION
  - –HIGH INTENSITY
  - –SEMI–MONOCHROMATIC CHARACTER

COUPLED WITH

- DEVELOPMENTS IN HARDWARE
  - –COMPUTING POWER
  - –DATA STORAGE
  - –DATA TRANSFER

COULD LEAD TO

NEAR REAL–TIME IMAGING

CONCLUSIONS
AND FUTURE DIRECTIONS

•DEMONSRATED:
- –SYNCHROTRON BASED MICROTOMOGRPHY
- –NEAR MICRON SCALE RESOLUTION
- –ELEMENTAL SPECIFICITY
- –QUANTITATIVE ANALYSIS CAPABILITY

•ANTICIPATE:
- –WIDE VARIETY OF DIAGNOSTIC APPLICATIONS
- –EXTENSION TO MICRON RESOLUTION
- –SCIENTIFIC APPLICATIONS IN INTERMEDITE LENGTH SCALE RANGE

•FUTURE DIRECTIONS:
- –DETECTOR IMPROVEMENTS
- –BEAMLINE CONSTRUCTION
  - X2 9/88
- –SPECIALIZED SAMPLES AND ENVIRONMENTS

LIQUID AND SOLID SURFACES†

P.S. Pershan
Physics Department & Div. of Applied Science
Harvard University

The use of specular reflection of X-rays to study the structure of the liquid-vapor and solid-vapor interfaces along the direction normal to the surface is described. If $R_F(\theta)$ is the theoretical Fresnel reflection law for x-rays incident on an ideal flat surface at an angle θ and $R(\theta)$ is the measured reflectivity from the true surface, the ratio $R(\theta)/R_F(\theta)$ is a measure of the electron density along the surface normal: i.e.

$$\frac{R(\theta)}{R_F(\theta)} \approx \left| \frac{1}{\rho_\infty} \int \left\langle \frac{\partial \rho(z)}{\partial z} \right\rangle e^{iQ_z z} dz \right|^2$$

where ρ_∞ is the electron density far from the surface, $\langle \partial\rho(z)/\partial z \rangle$ is the average gradient of the electron density along the surface normal and $Q_z=(4\pi/\lambda)\sin(\theta)$. Experimental results will be presented for: i) the surface of simple liquids; ii) smectic order induced on the surface of certain liquid crystals ; iii) structure on the surface of micellar phases; and iv) organic coatings on silicon.

† The research reported here was supported by the U.S. National Science Foundation through Grant NSF-DMR-85-13523, through the Harvard Materials Research Laboratory, Grant Number NSF-DMR-86-14003 and by the Joint Services Electronics Program through grant N00014-75-C-0648.

User's Meeting for the Advanced Photon Source
Argonne National Laboratory, March 9-10, 1988

LIQUID AND SOLID SURFACES

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Physics Department & Div. of Applied Science
Harvard University

HARVARD: PHYSICS
Alan Braslau, Dan Schwartz, Gerry Swislow, Ian Tidswell, Alex Weiss

HARVARD: CHEMISTRY
George Whitesides, Roy Gordon, Steve Wasserman

BROOKHAVEN NATIONAL LABORATORY
John Axe, Ben Ocko

RISO NATIONAL LABORATORY DENMARK
Jens Als-Nielsen

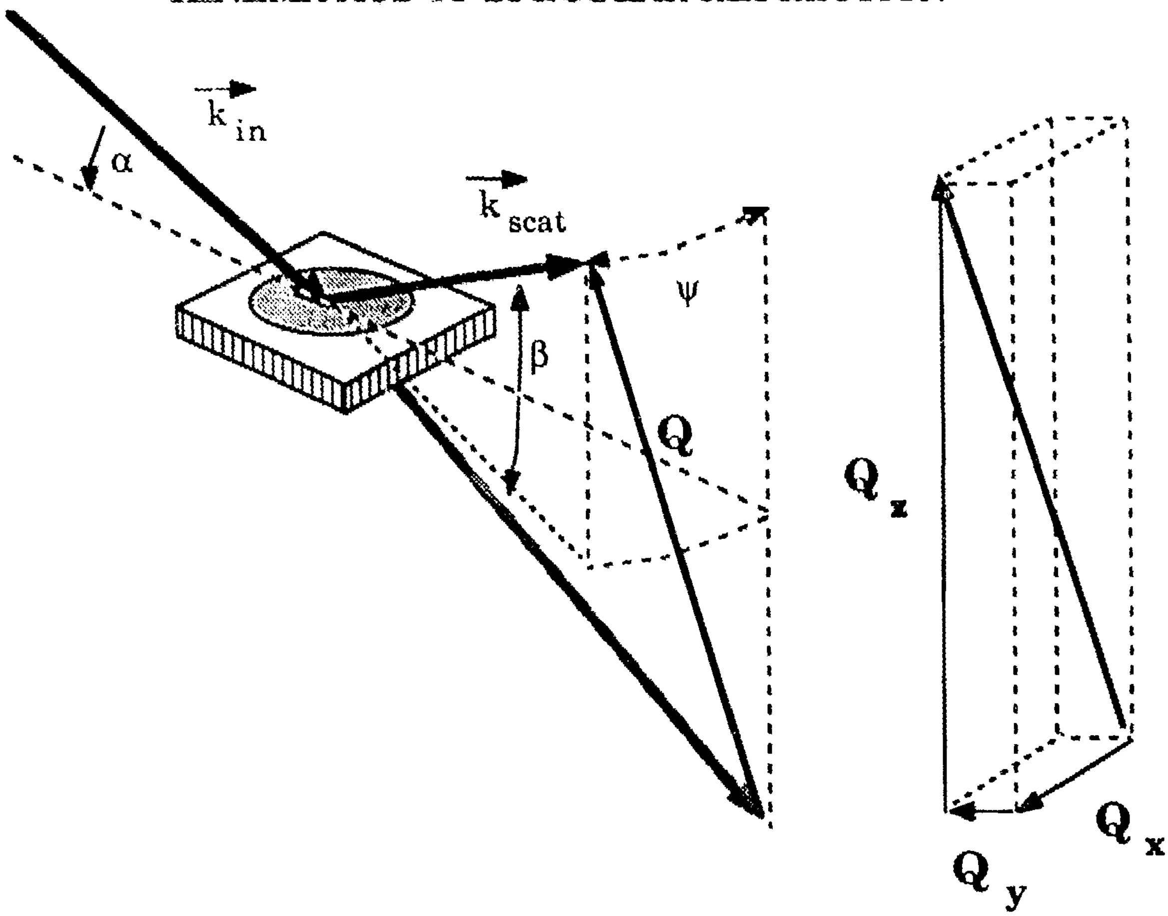
BAR-ILAN UNIVERSITY, ISRAEL
Moshe Deutsch

EXXON CORPORATE RESEARCH LABORATORY
John Huang

OUTLINE

SPECULAR REFLECTION:
Basic Ideas
Examples: Simple Liquids H_2O, CCl_4, CH_3OH
Liquid Crystals
Micellar Materials
Solid Surfaces
DIFFUSE SCATTERING FROM SURFACES
PROBLEMS AND POSSIBILITIES

KINEMATICS OF SPECULAR REFLECTION



SPECULAR REFLECTION: $\alpha = \beta$ and $\psi = 0$

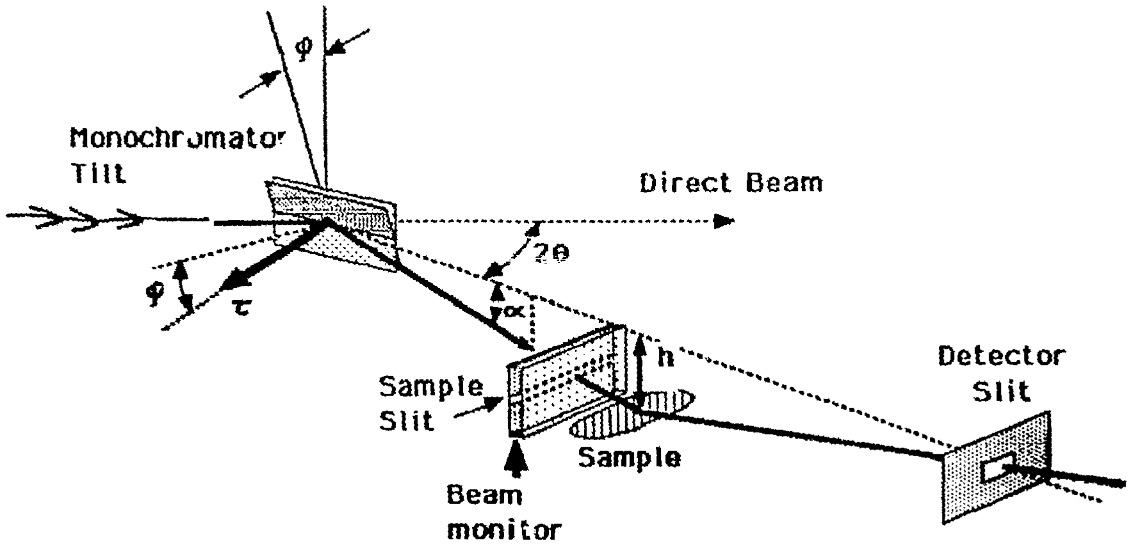
$$Q_x = Q_y = 0 \text{ and } Q_z = \frac{4\pi}{\lambda}\sin(\alpha)$$

DIFFUSE SCATTERING:

$$\alpha \neq \beta \Rightarrow Q_y \approx \frac{Q_z}{2}[\beta - \alpha] \approx \frac{2\pi}{\lambda}\alpha[\beta-\alpha] \qquad \psi \neq 0 \Rightarrow Q_x \approx \frac{4\pi}{\lambda}\cos(\alpha)\frac{\psi}{2}$$

SPECULAR REFLECTION GEOMETRY

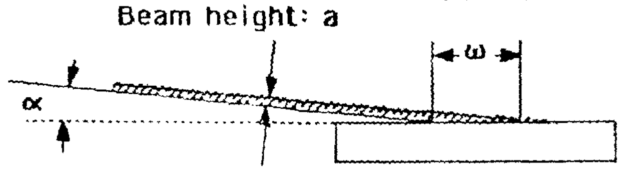
FOR SYNCHROTRON RADIATION



$(k_I)_z = \tau \sin(\varphi) = (2\pi/\lambda)\sin(\alpha)$

Coupling of λ and θ $\quad (\lambda\tau/2\pi)^2 = 2[1-\cos(\alpha)\cos(2\theta)]$

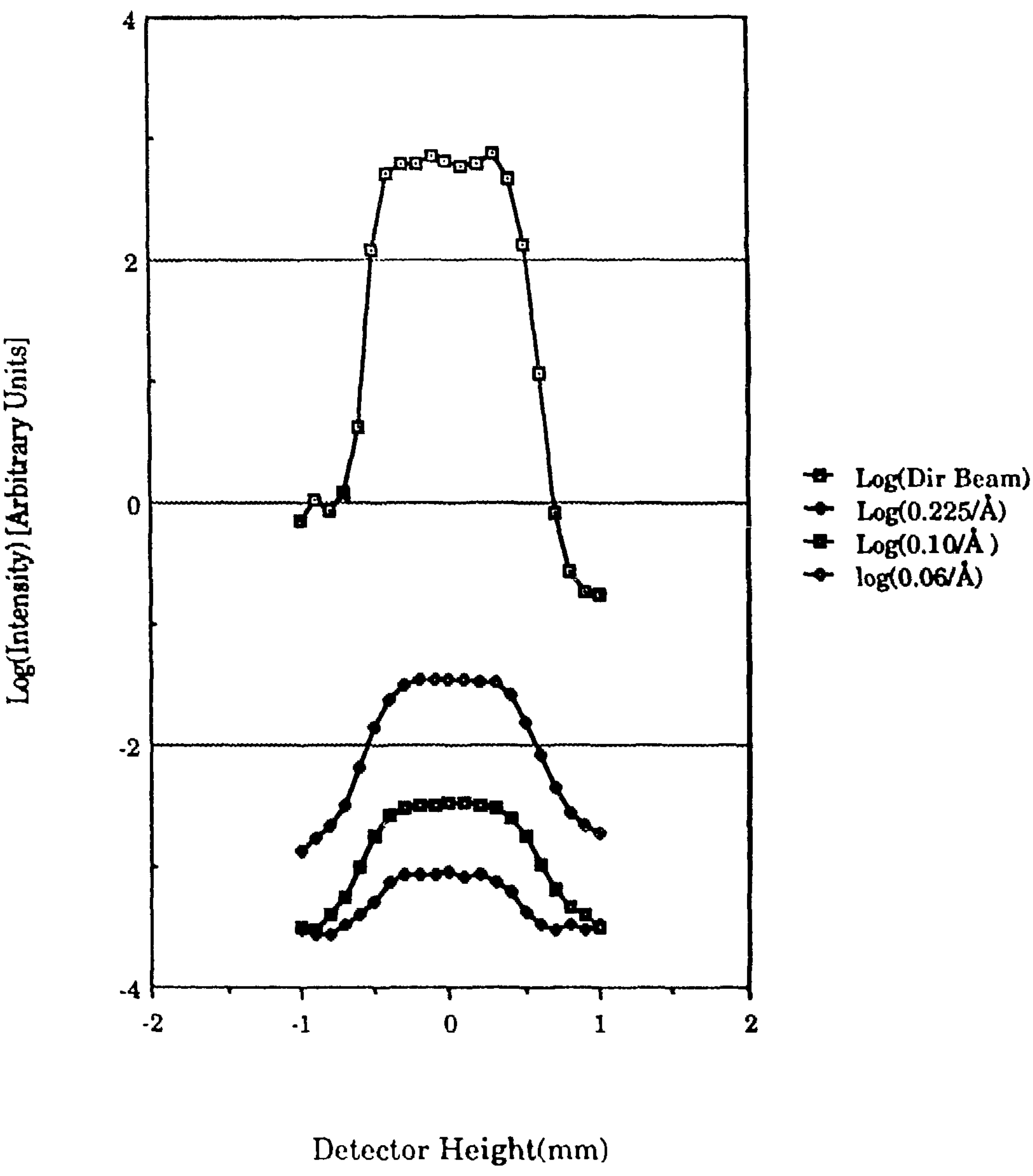
"Foot Print" on Sample



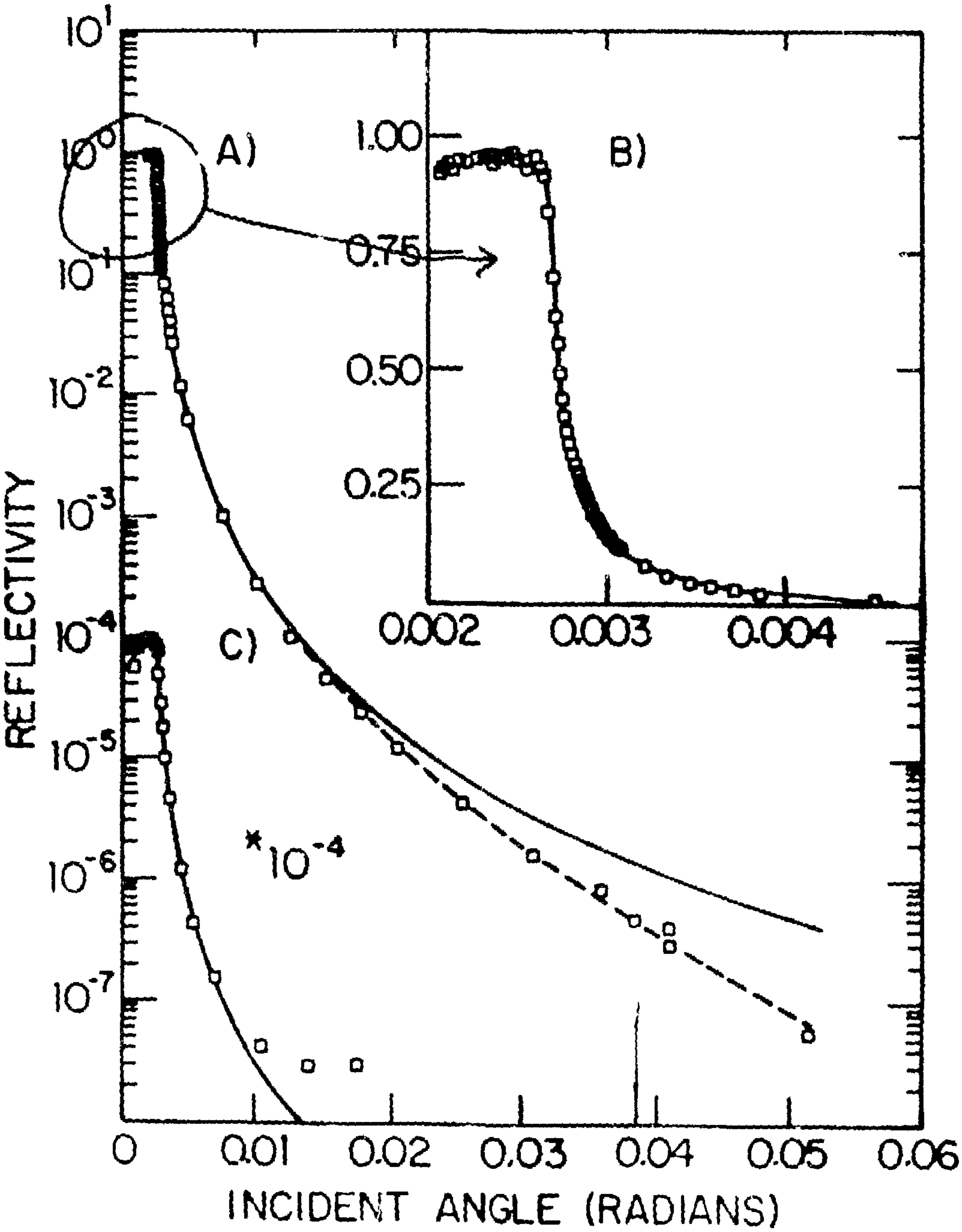
$\omega = a/\sin(\alpha)$

If $\alpha = 0.1^0$ then $\omega \approx 600 * a$

Detector Height Scans At Varying Qz



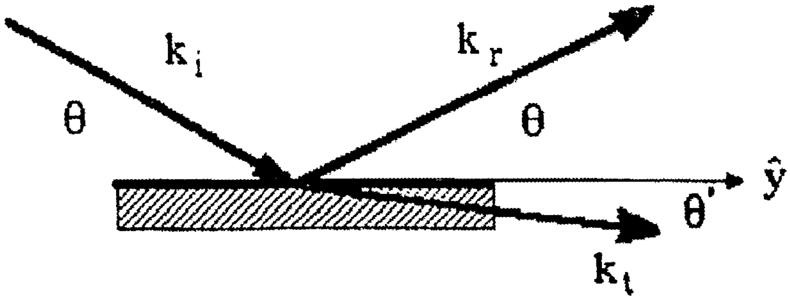
J Als-Nielsen, A. Braslau, M. Deutsch, A. Weiss
+ P.S.P
JULY 1984 : DESY [Phys Rev. Lett. 54, 114 (1985)]



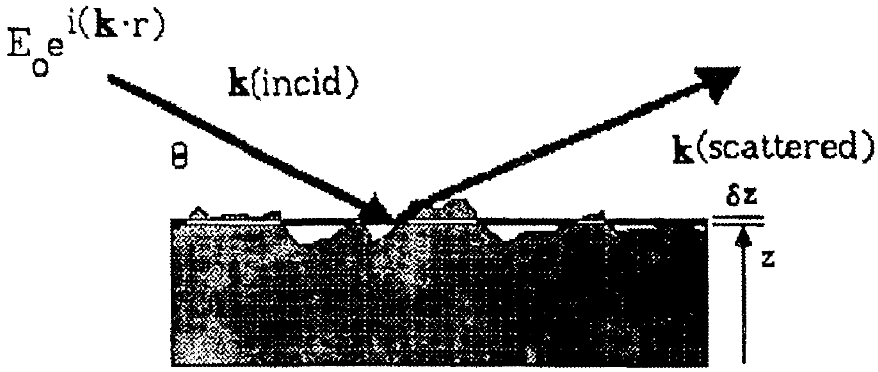
SPECULAR REFLECTION FROM AN IDEAL FLAT SURFACE

Dielectric constant

$$\varepsilon = 1 - \frac{\rho r_e^2 \lambda^2}{\pi} \approx 1 - \theta_c^2$$



$$R_F(\theta) = \left\{ \frac{\sin(\theta) - \sqrt{\varepsilon - \cos^2(\theta)}}{\sin(\theta) + \sqrt{\varepsilon - \cos^2(\theta)}} \right\}^2 \approx \left(\frac{\theta_c}{2\theta} \right)^4 \text{ for } \theta >> \theta_c$$



$$\frac{E_s}{E_o} \propto \int [\rho(x,y,z)\delta z] e^{i[\mathbf{k}_{in} - \mathbf{k}_{scat}] \bullet \mathbf{r}} dxdy$$

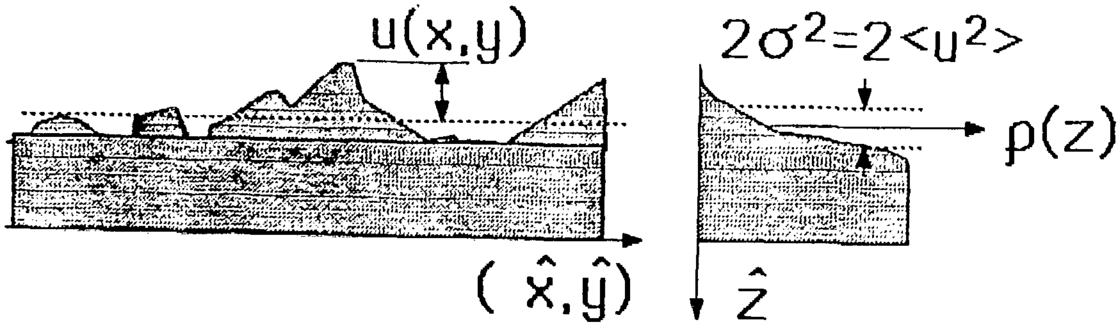
$$\propto \delta z \left[<\rho(z)> \delta^2(\mathbf{Q}_{x,y}) + S(z, Q_{x,y}) \right] e^{iQ_z z}$$

Specular reflection is obtained from the leading term!!

for $\theta >> \theta_c$

$$\boxed{\frac{R(\theta)}{R_F(\theta)} \approx \left| \frac{1}{\rho_\infty} \int \left< \frac{\partial \rho(z)}{\partial z} \right> e^{iQ_z z} dz \right|^2}$$

DENSITY PROFILE



If: $(1/\rho)\partial\langle\rho\rangle/\partial z=(1/\sqrt{2\pi\sigma^2})\exp(-z^2/2\sigma^2)$

THEN: $R(Q)/R_F(Q)=\exp(-Q^2\sigma^2)$

H_2O, CCl_4, etc"Debye-Waller"

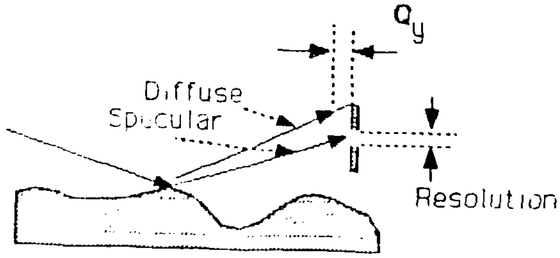
surface energy/unit area

$$U\approx(\gamma/2)\{\nabla_\perp u\}^2$$

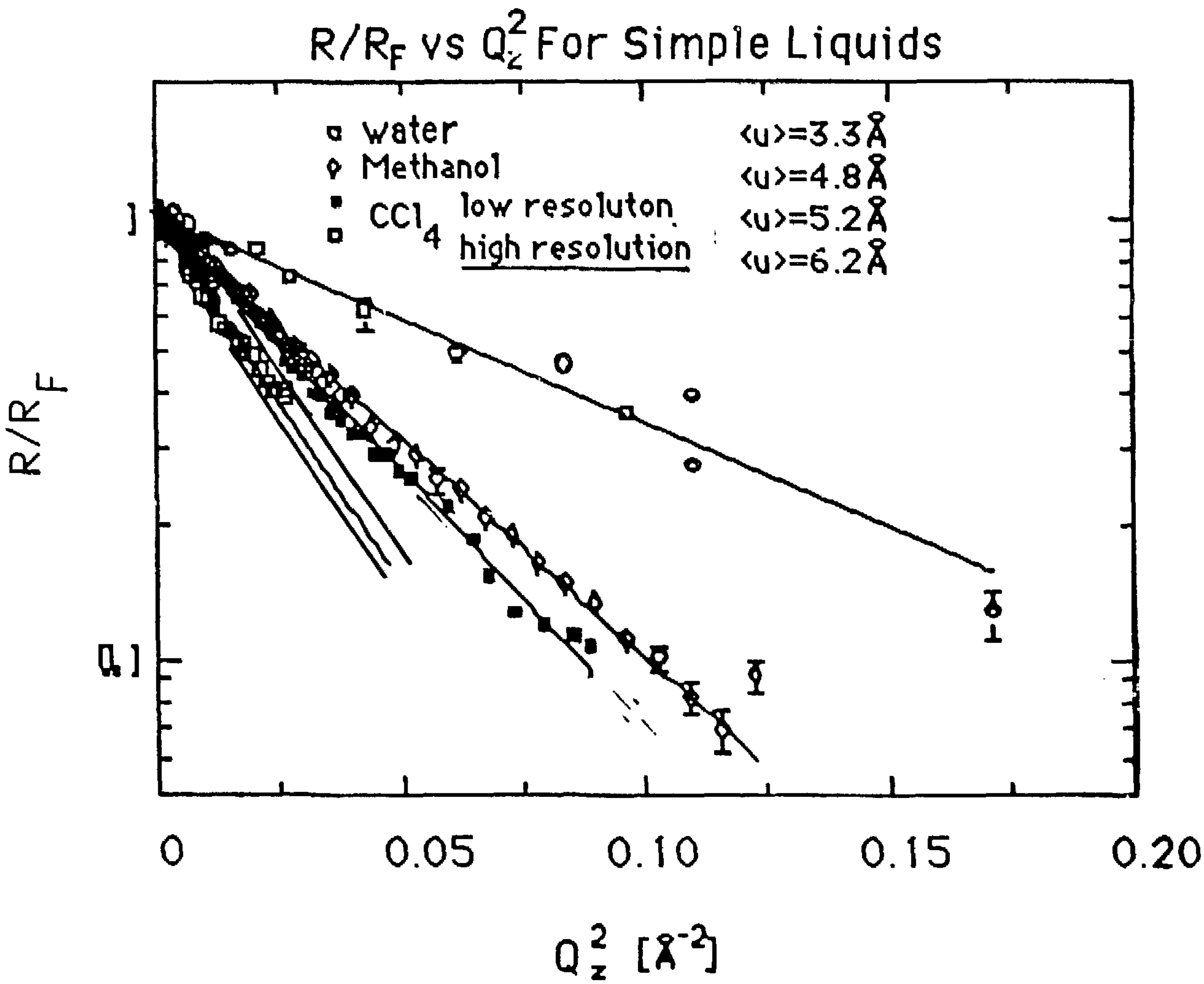
$$\sigma^2=(k_BT/\gamma 4\pi^2)\int_{L_1}^{L_2} d^2q/q^2 \;\propto\; \ln(L_2/L_1)$$

$L_2=\pi/$molecular size

$L_1=1/$resolution$\approx 10^{-4}$ Å^{-1}



$$\text{Log}\ \frac{R(Q_z)}{R_F(Q_z)} = -\langle u\rangle^2\ Q_z^2$$



ROUGHNESS OF LIQUID SURFACES

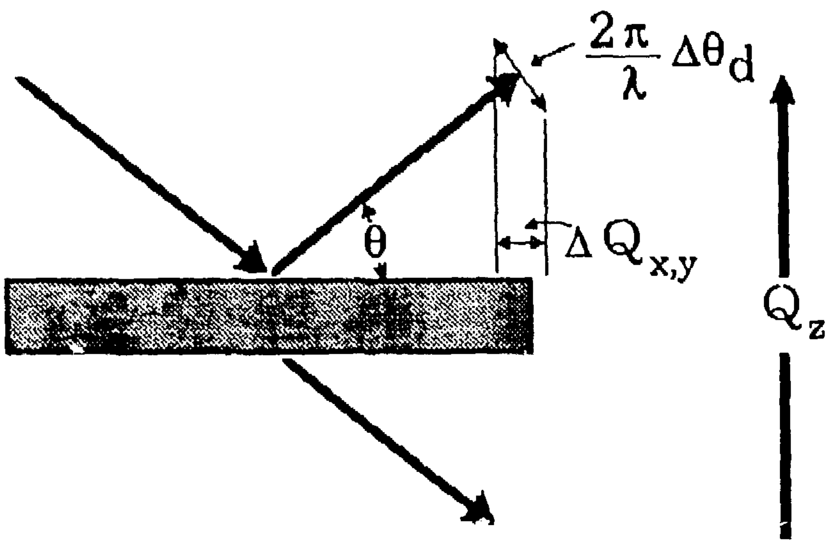
Contribution From Capillary Waves:

$$\sigma_c^2(Q_z) = \frac{k_B T}{2\pi\gamma} \log_e\left(\frac{2\pi}{Q_z r_m(\Delta\theta_d)}\right)$$

where

upper limit of integral is $\approx \pi/r_m$ (r_m= radius of molecule)

lower limit of integral is $\approx \frac{2\pi}{\lambda}\theta\Delta\theta_d \approx \frac{Q_z}{2}\Delta\theta_d$



$\sigma_c^2(Q_z)$ depends on : 1-Height of detector slit (i.e. resolution)

2-Incident angle (Q_z)

3-Surface tension of liquid

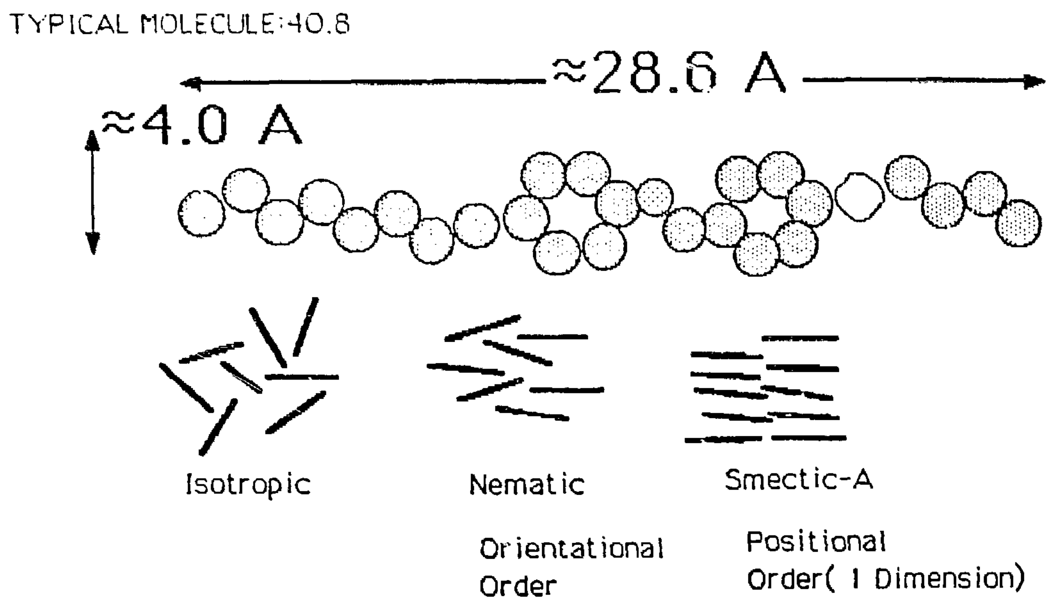
Total Roughness: $\sigma_T^2(Q_z) = \sigma_c^2(Q_z) + \sigma_I^2$

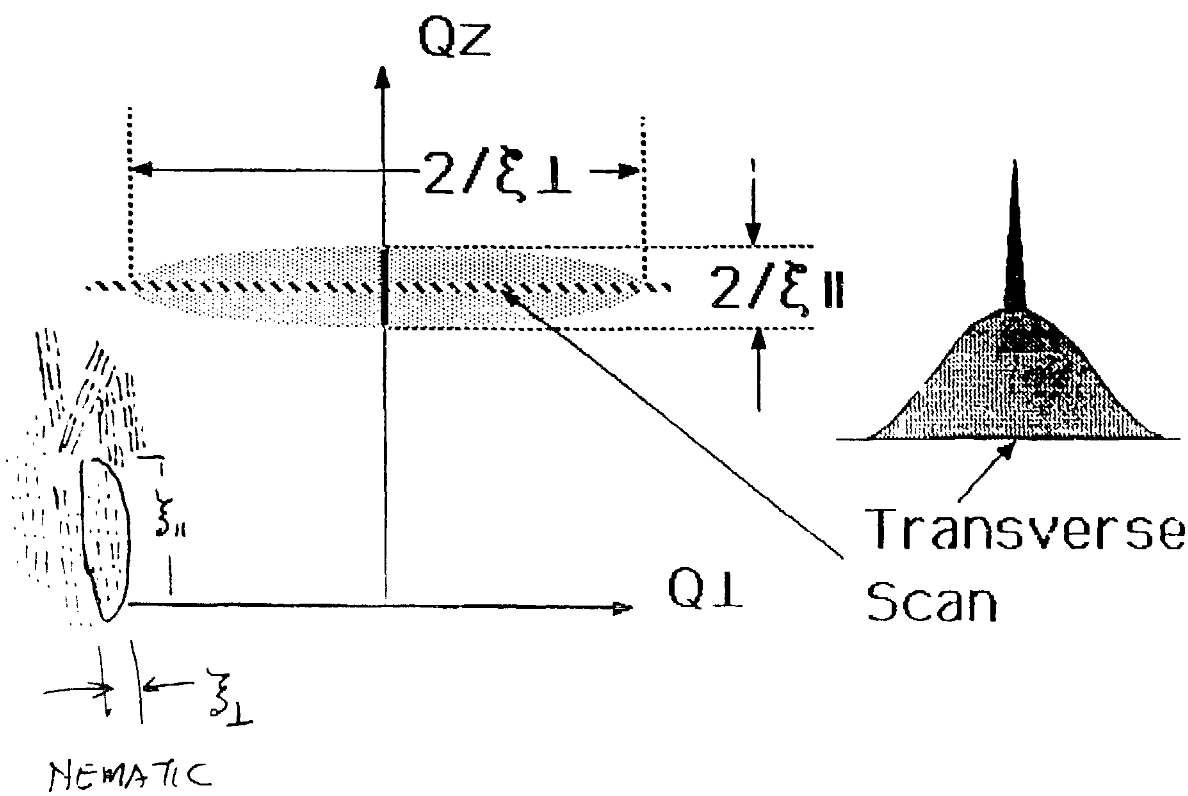
where σ_I is the "intrinsic" width of the profile.

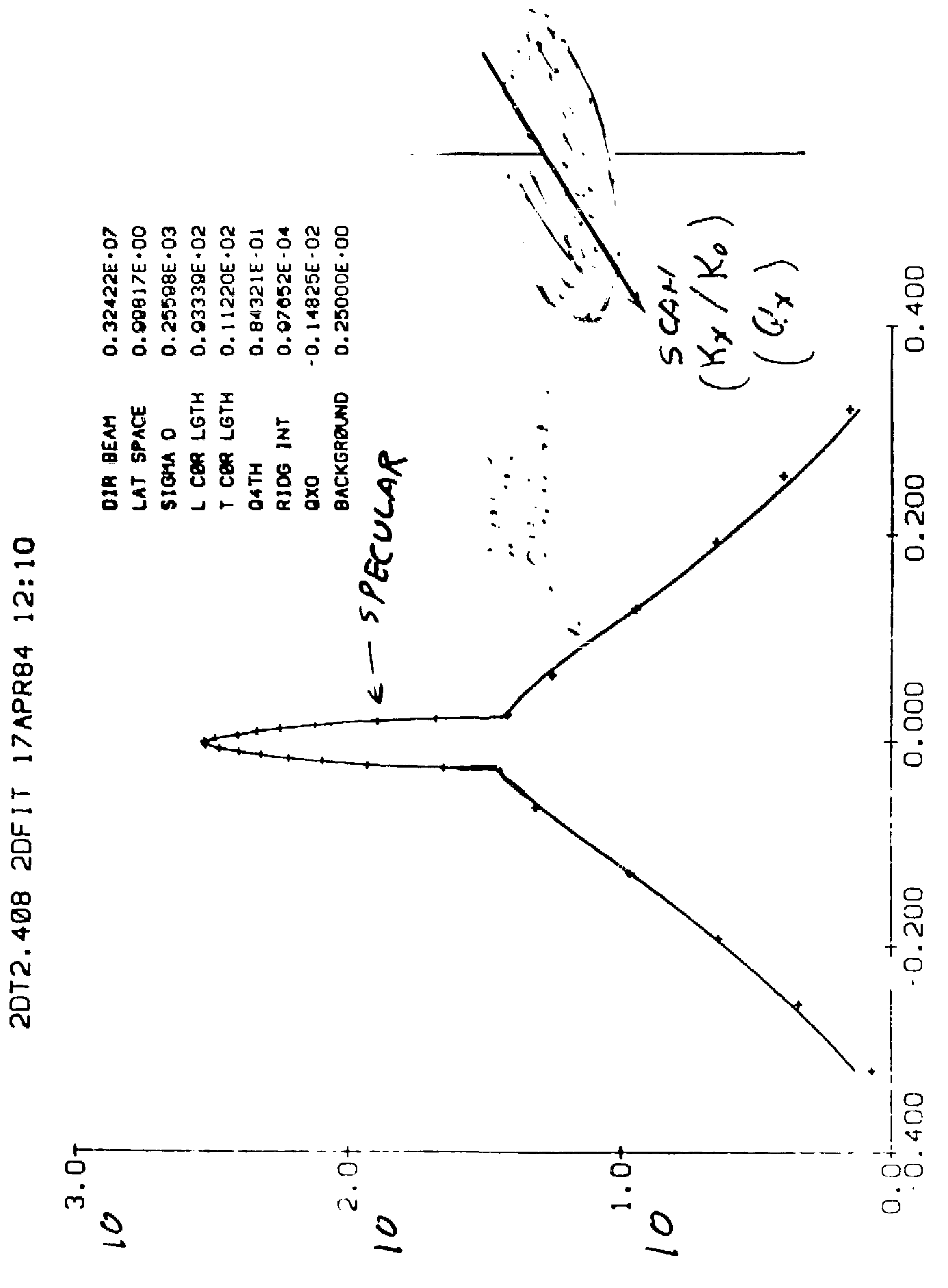
RESULTS

Resol.	sample	r_m	γ	$\sigma_c(0.4Å^{-1})$	σ_T(measured)	$\Rightarrow \sigma_I$
		(Å)	(dynes/cm)	(Å)	(Å)	(Å)
	H_2O	**1.93**	73	2.77	3.3	**1.8±0.2**
Low	CCl_4	**3.38**	27	4.83	5.9	**3.4±0.1**
High	"			4.41	5.1	**2.6±0.1**
	CH_3OH	**2.52**	23	4.65	4.8	**1.2±0.4**

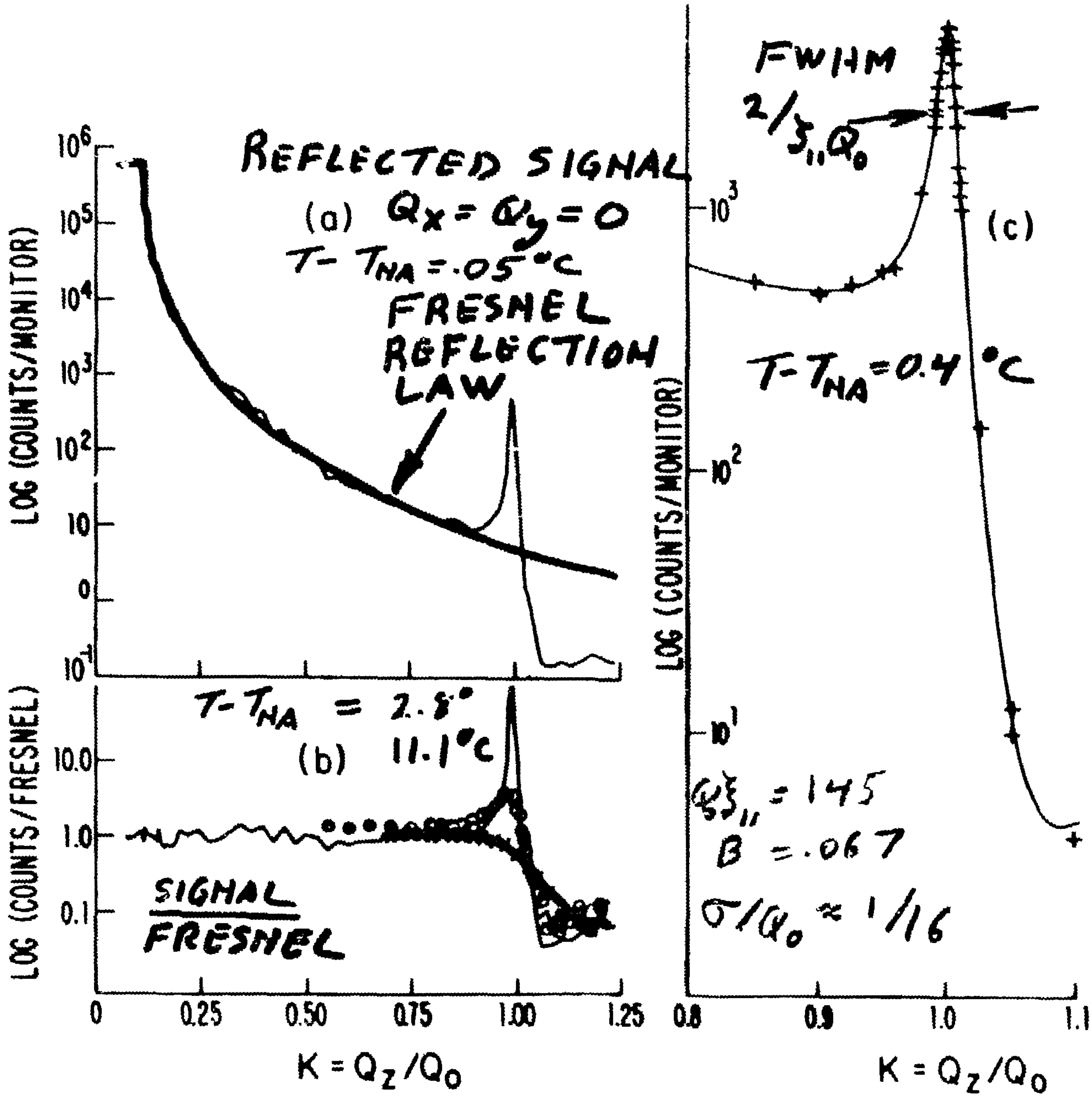
LIQUID CRYSTALS





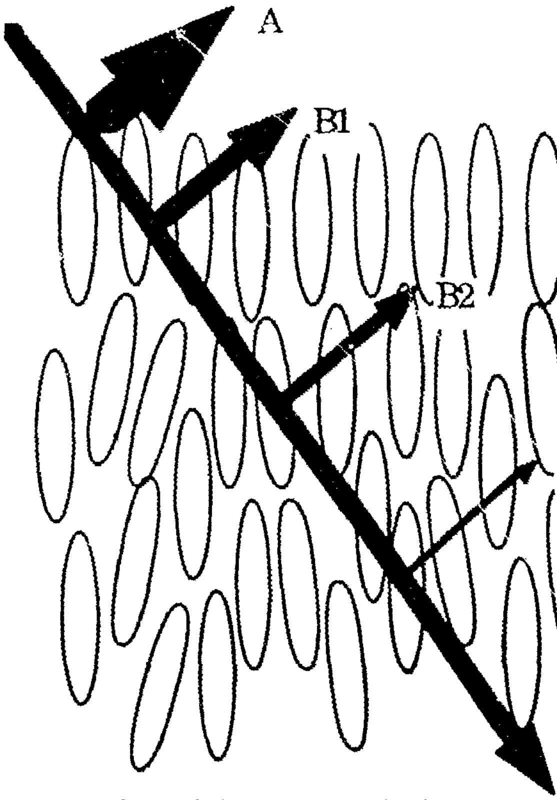

2DT2.408 2DFIT 17APR84 12:10
DIR BEAM 0.32422E-07
LAT SPACE 0.99817E-00
SIGMA 0 0.25598E-03
L COR LGTH 0.93339E-02
T COR LGTH 0.11220E-02
Q4TH 0.84321E-01
RIDG INT 0.97652E-04
QX0 -0.14825E-02
BACKGROUND 0.25000E-00
← SPECULAR
SCAN
(Kx / K0)
(Qx)
10 3.0
10 2.0
10 1.0
0.0
-0.400
-0.200
0.000
0.200
0.400
KX/K0

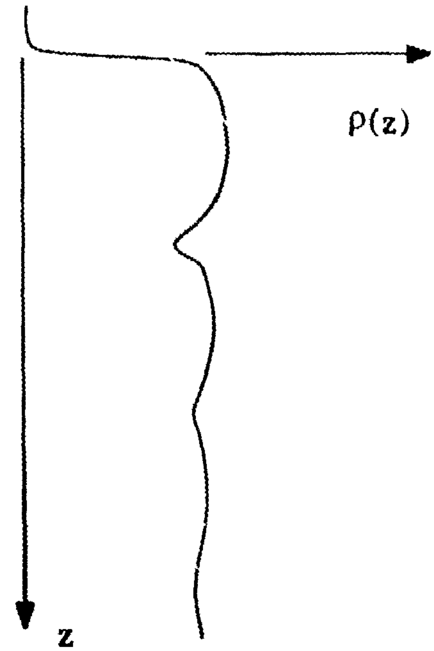
8OCB



$K = \sin\theta / \sin\theta_0$

SURFACE INDUCED SMECTIC-A ORDER





REFELECTED SIGNAL:

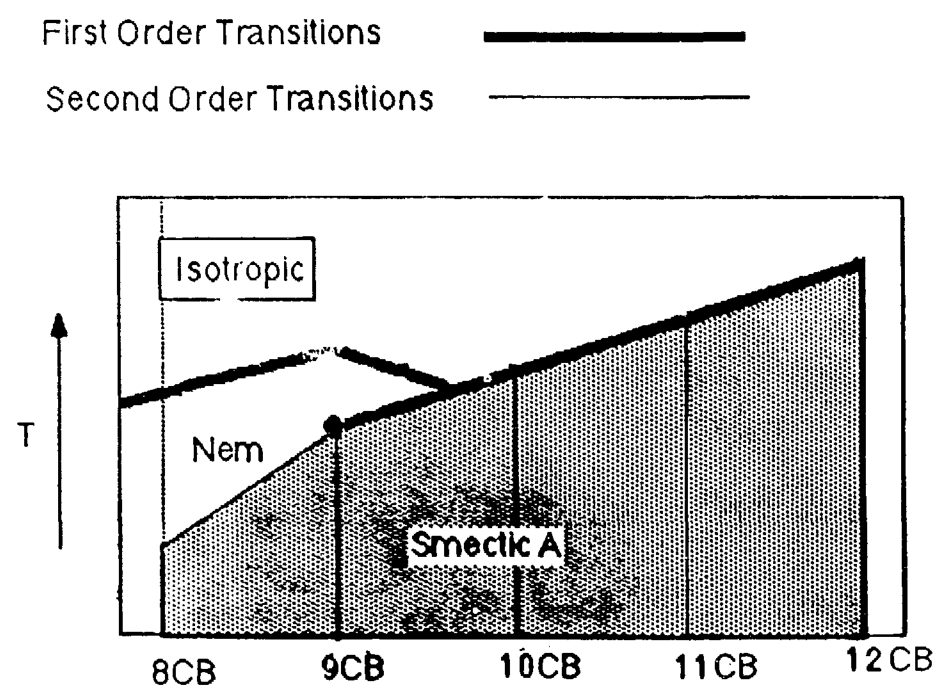
$$\left| A(Q) + \sum_{n=1}^{\infty} Bn(Q)e^{iQ(nd)} \right|^2 \qquad \text{where } Q = \frac{4\pi}{\lambda}\sin(\theta).$$

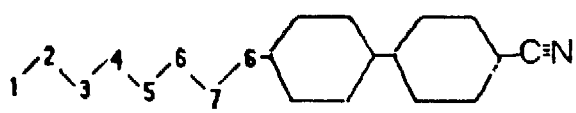
$$\text{If } Bn \sim e^{-nd/\xi} \Rightarrow \sum_{n}^{\infty} e^{-nd[1/\xi - iQ]}$$

$\Rightarrow$ Lorentzian peaked at $Q \sim \frac{2\pi}{d}$ with a HWHM $\Delta Q \sim \frac{1}{\xi}$

nCB PHASE DIAGRAM

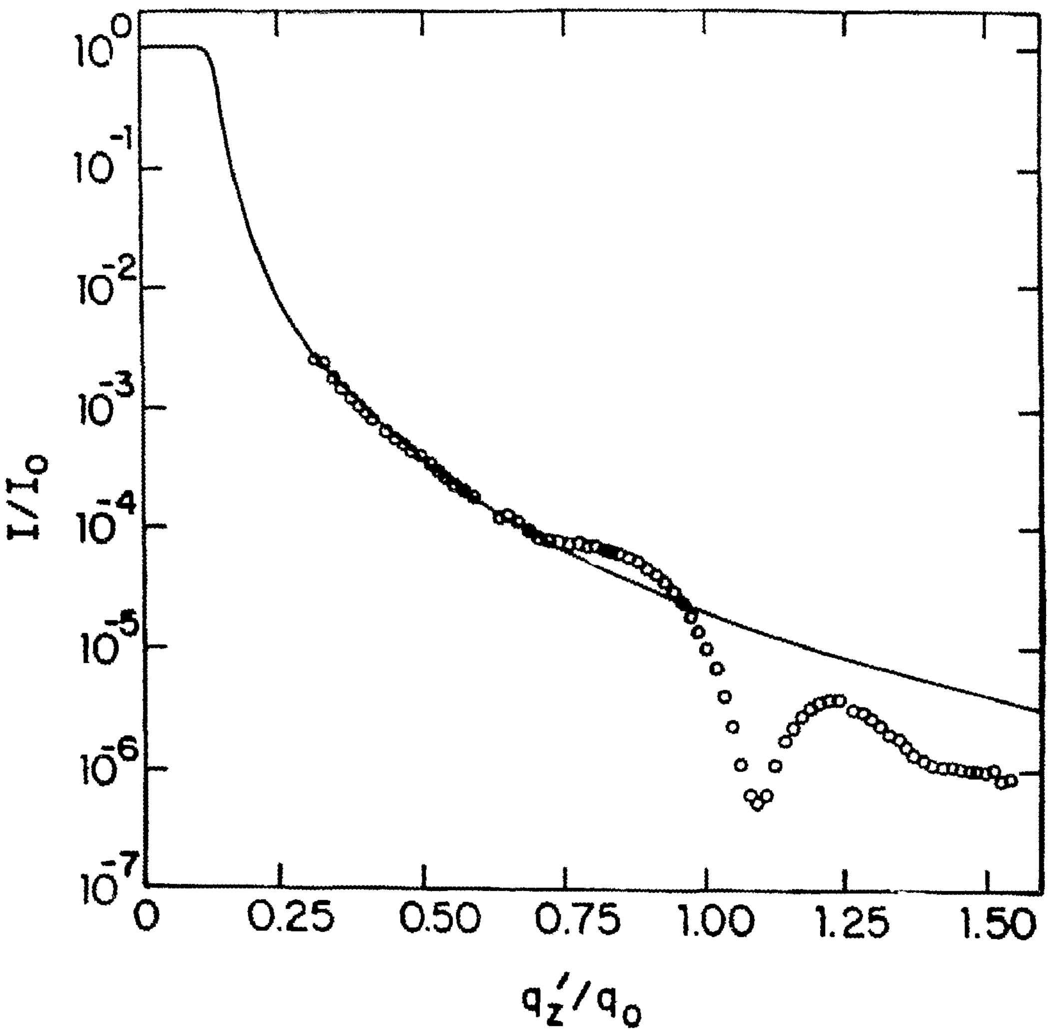
J. Thoen, H. Marynissen, W. Van Dael, Phys. Rev. Lett. 52,204(1984)





8CB

REFLECTION FROM THE ISOTROPIC VAPOR INTERFACE of 12CB



Nematic to Smectic-A

exponential density oscillations

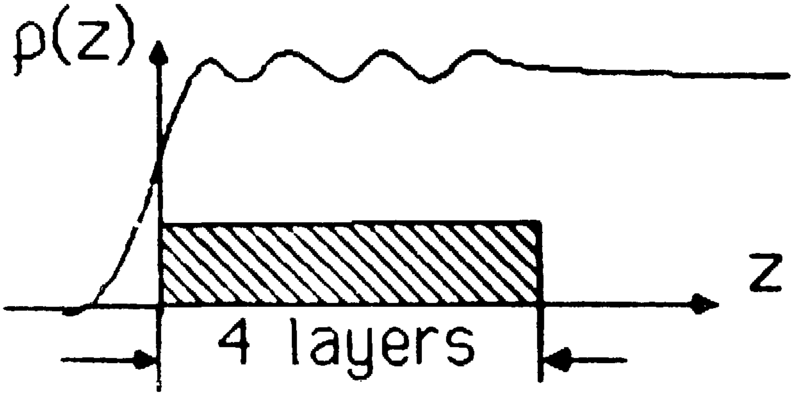
$$\sin(Q_0 z + \phi)\cdot\exp(-z/\xi_{\parallel})$$

Lorentzian Fourier transform

$$\approx 1/[1 + (\xi_{\parallel})^2(Q-Q_0)^2]$$

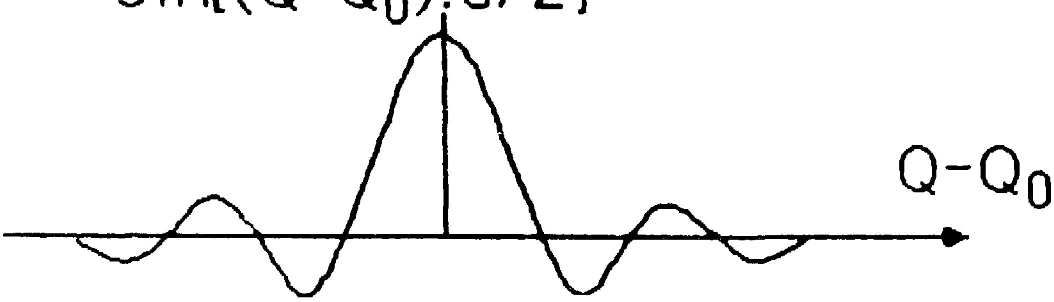
Isotropic to Smectic-A

Finite number of periods



Fourier Transform of Square Wave

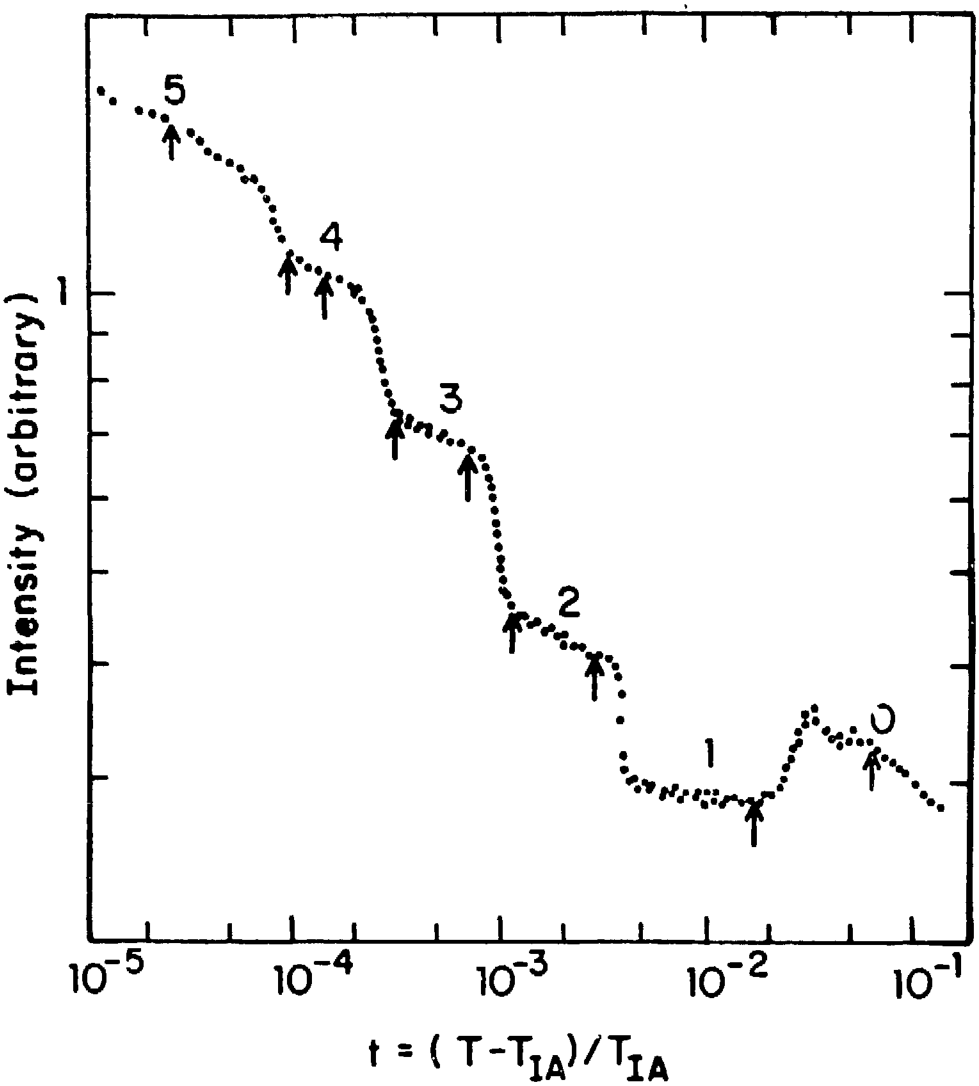
$$\frac{\sin[(Q-Q_0)\cdot nd/2]}{\sin[(Q-Q_0).d/2]}$$



Ben Ocko, Alan Braslau
J. Als-Nielsen, M. Deutsch

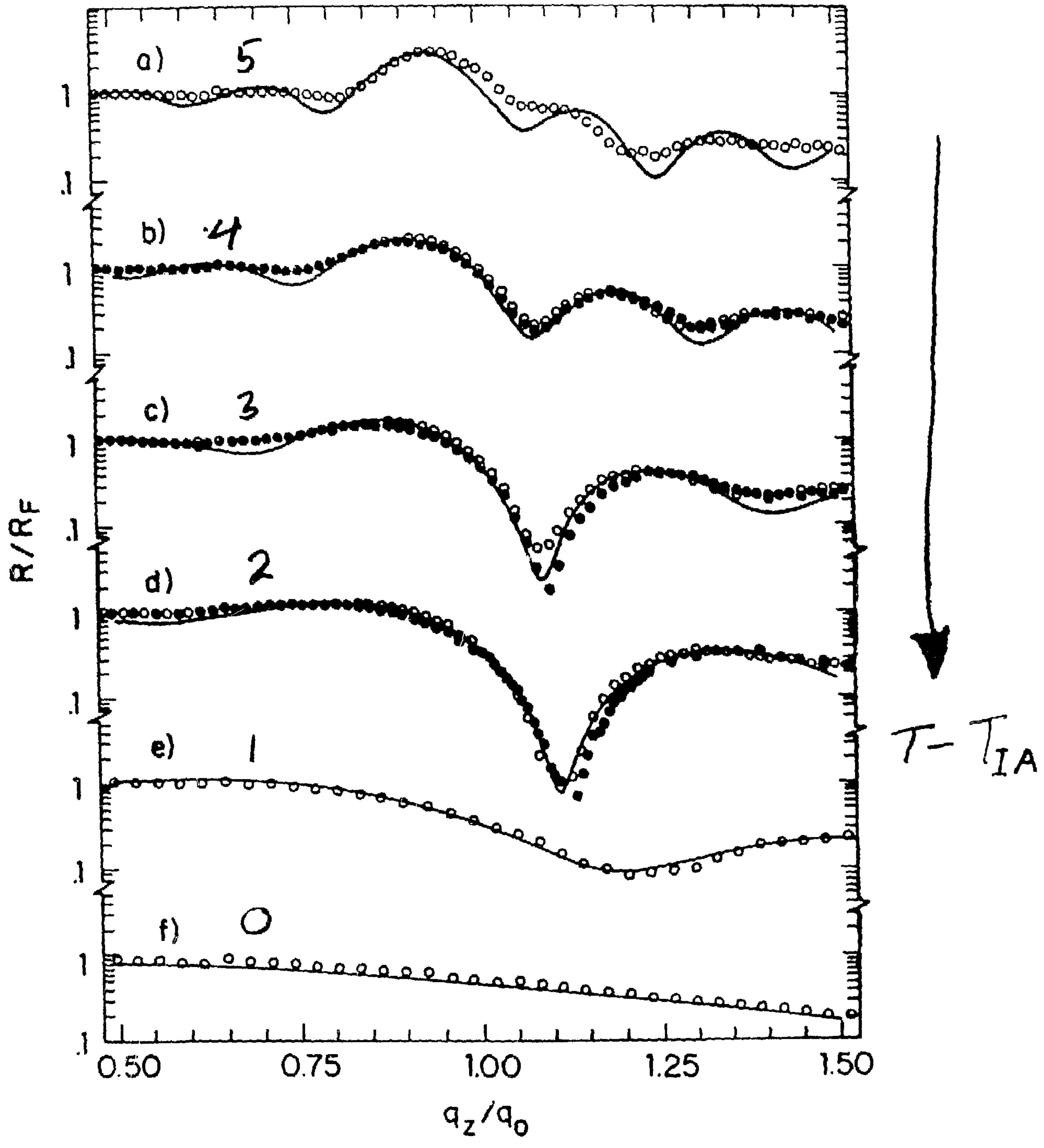
12CB ISOTROPIC PHASE

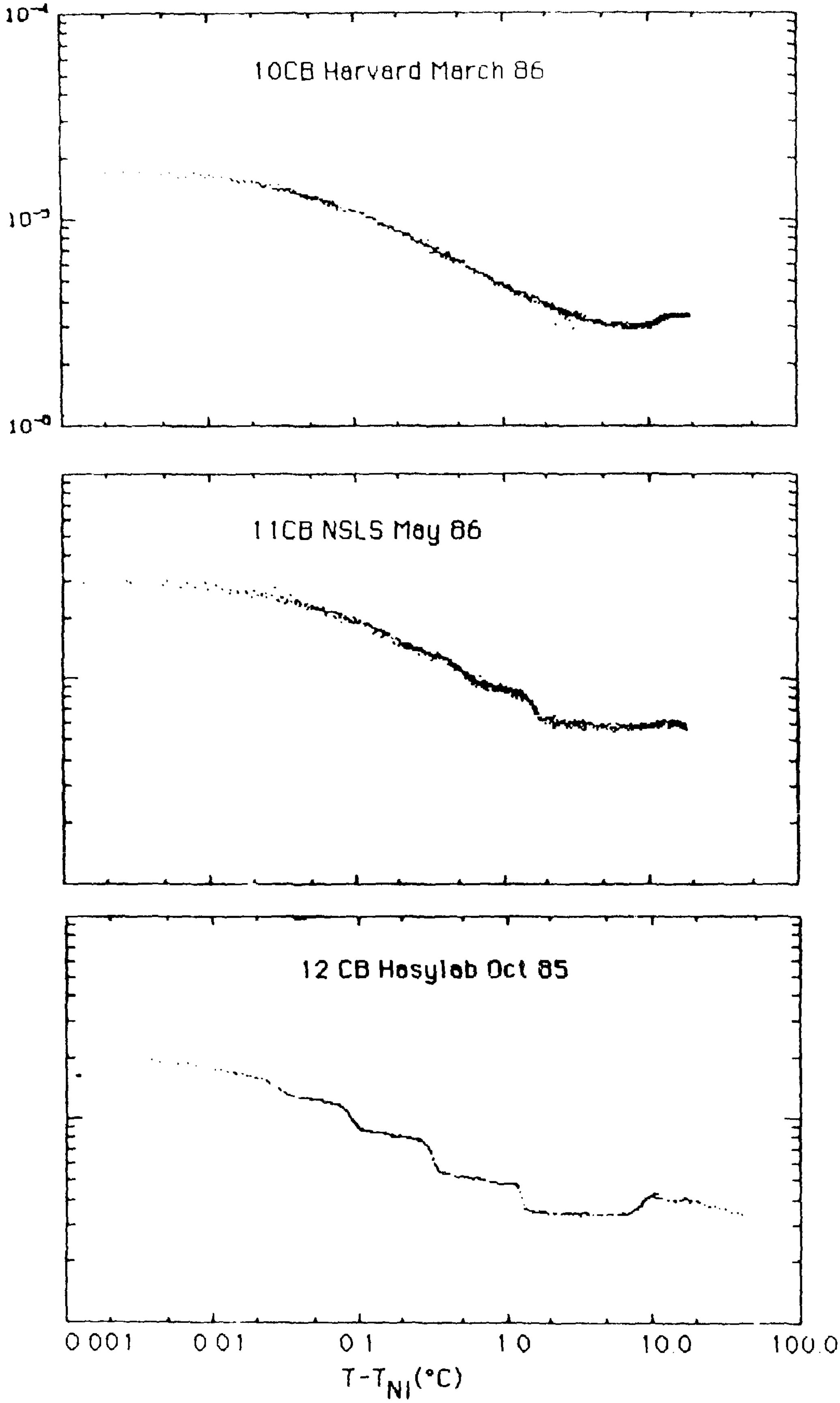
R(Q)/R_F(Q)

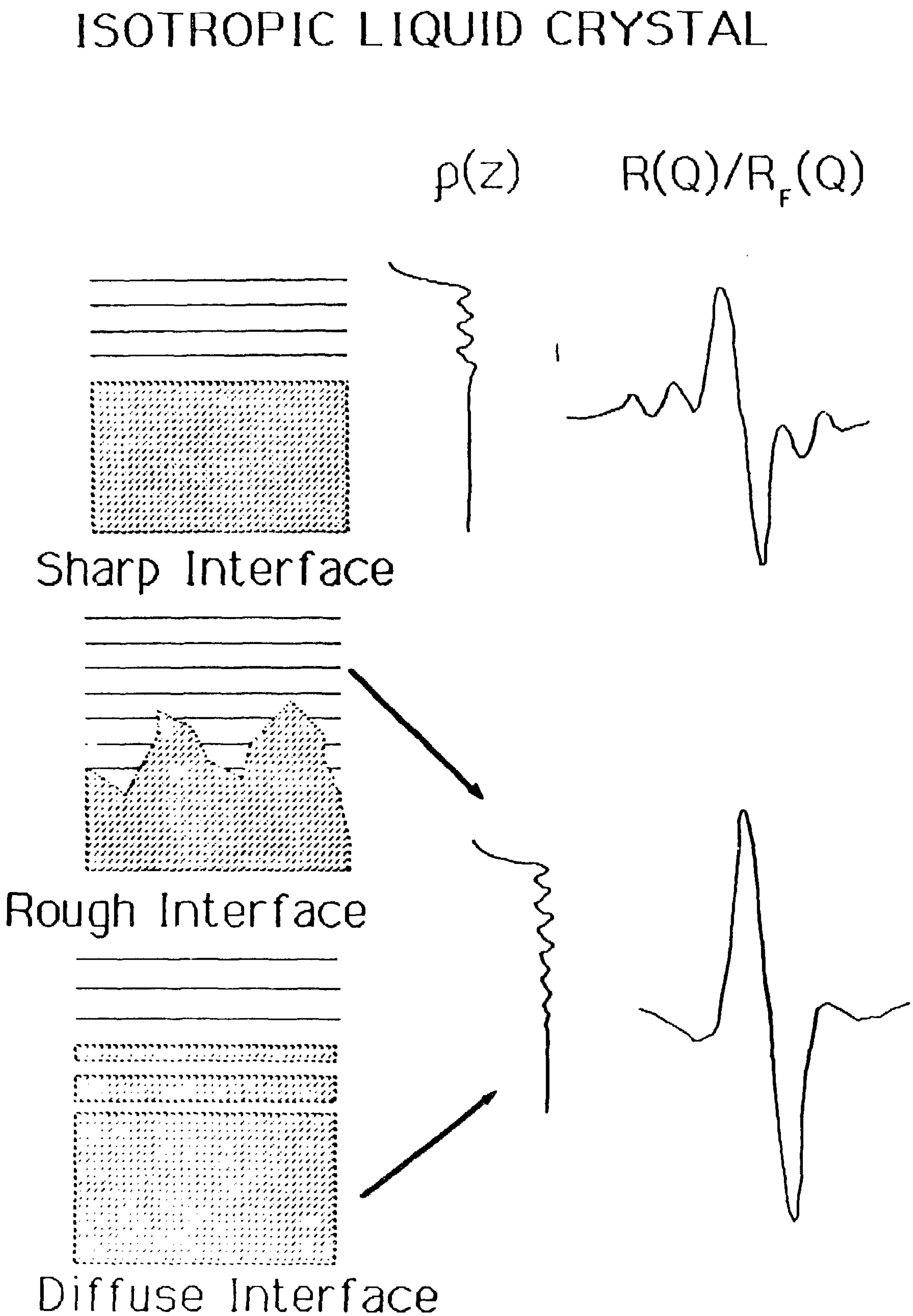


Ocko, Braslau, Als-Nielsen, Deutsch
P.R. Lett. 57, 94 (1986)

12CB

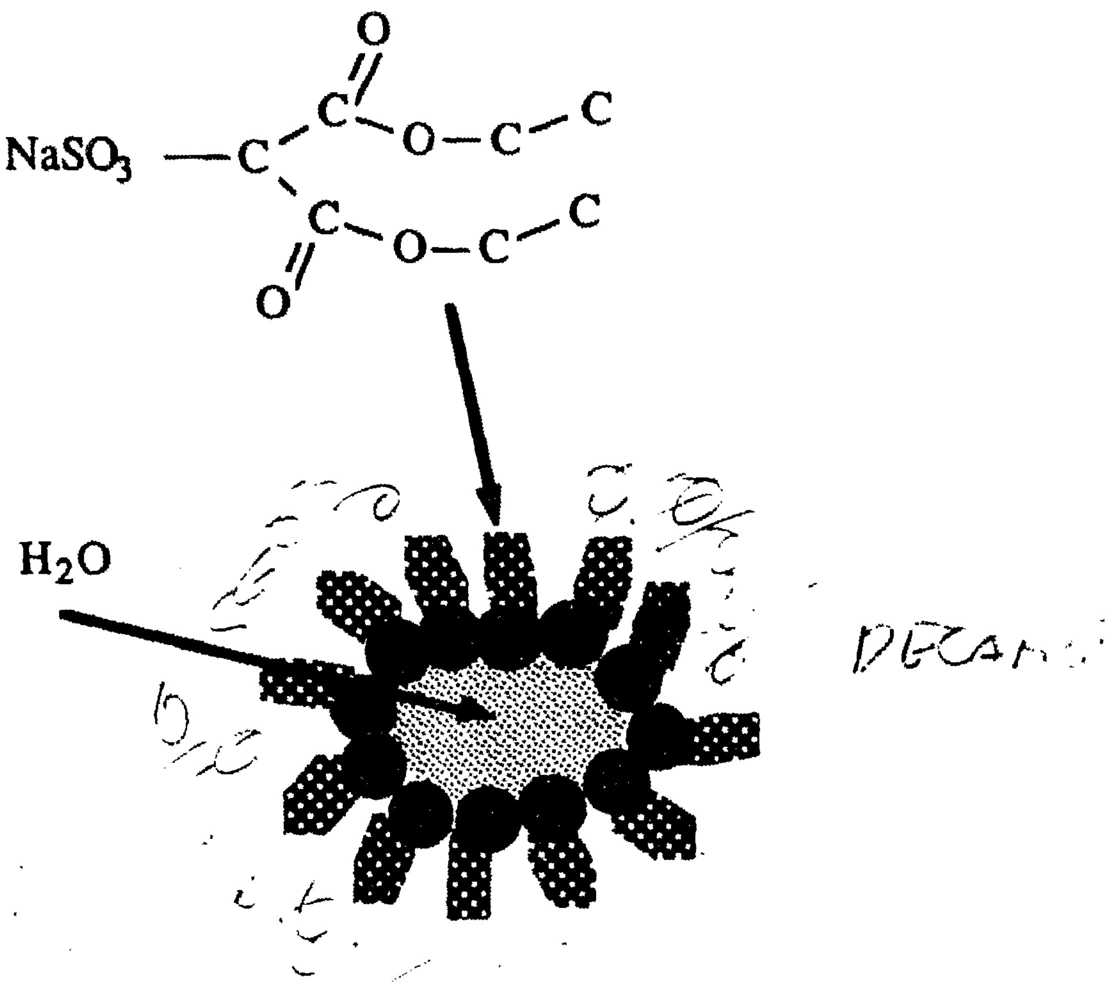



10CB Harvard March 86
11CB NSLS May 86
12 CB Hasylab Oct 85
0.001
0.01
0.1
1.0
10.0
100.0
T-T$_{NI}$(°C)


ISOTROPIC LIQUID CRYSTAL
ρ(z)
$R(Q)/R_F(Q)$
Sharp Interface
Rough Interface
Diffuse Interface

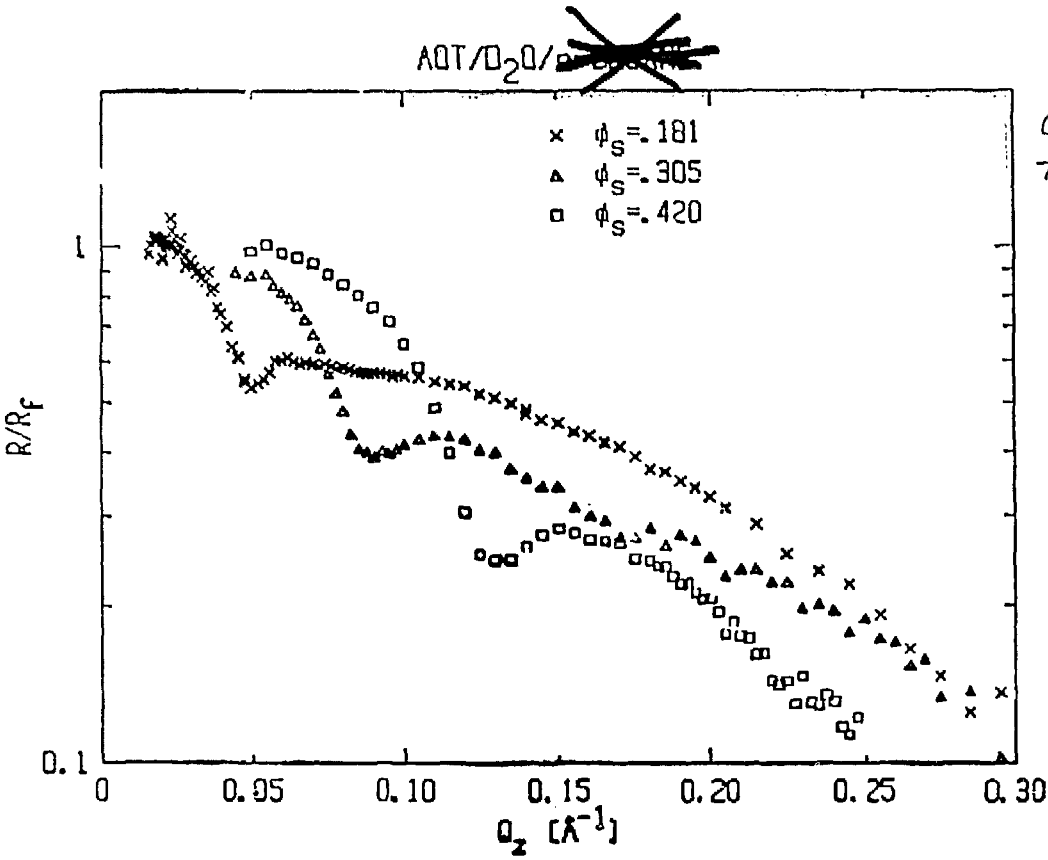
REPRODUCED FROM BEST
AVAILABLE COPY

AOT

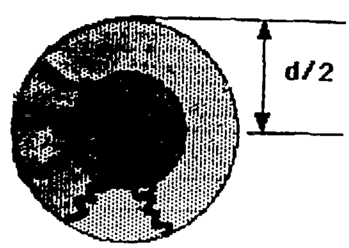


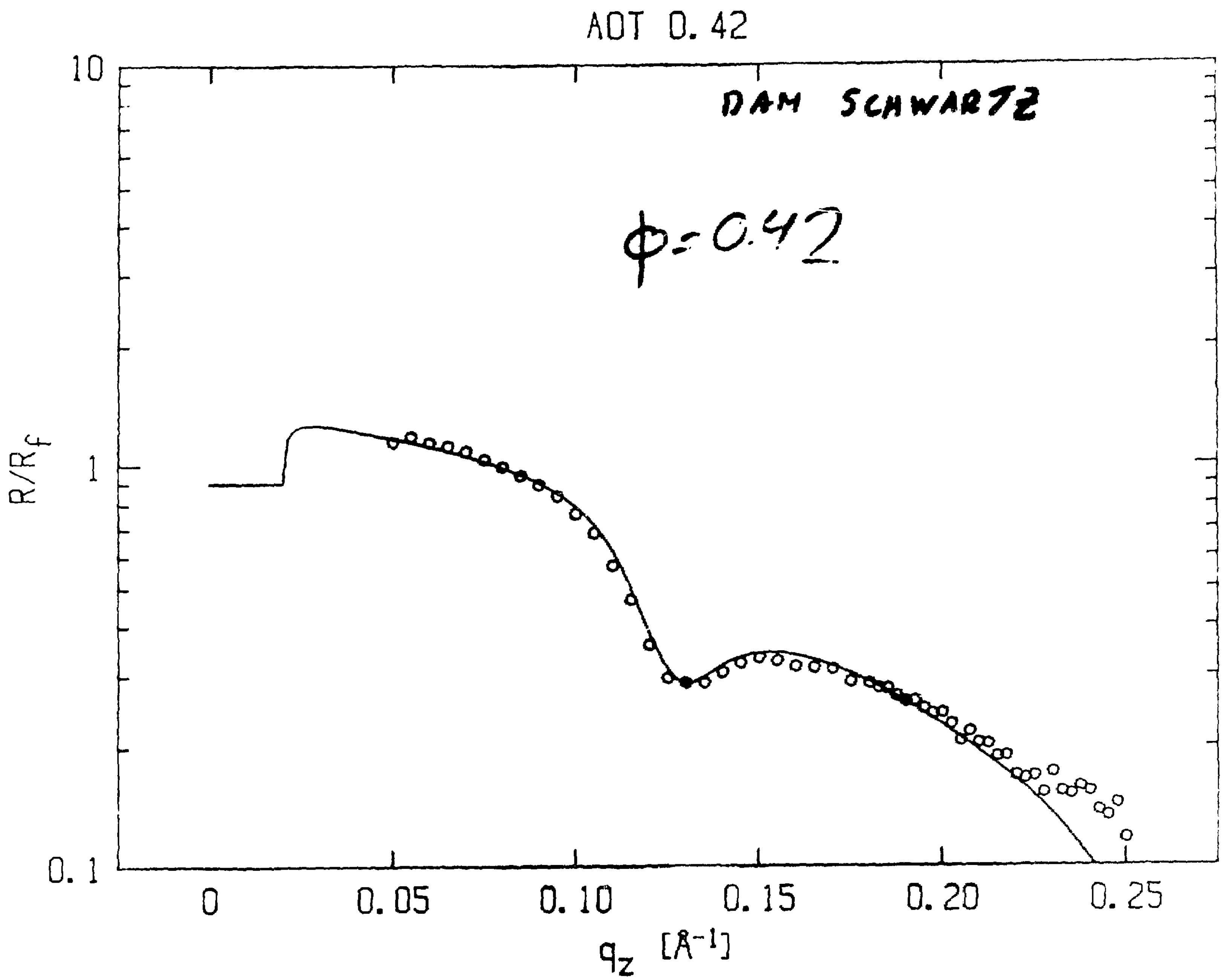
AOT MICELLE

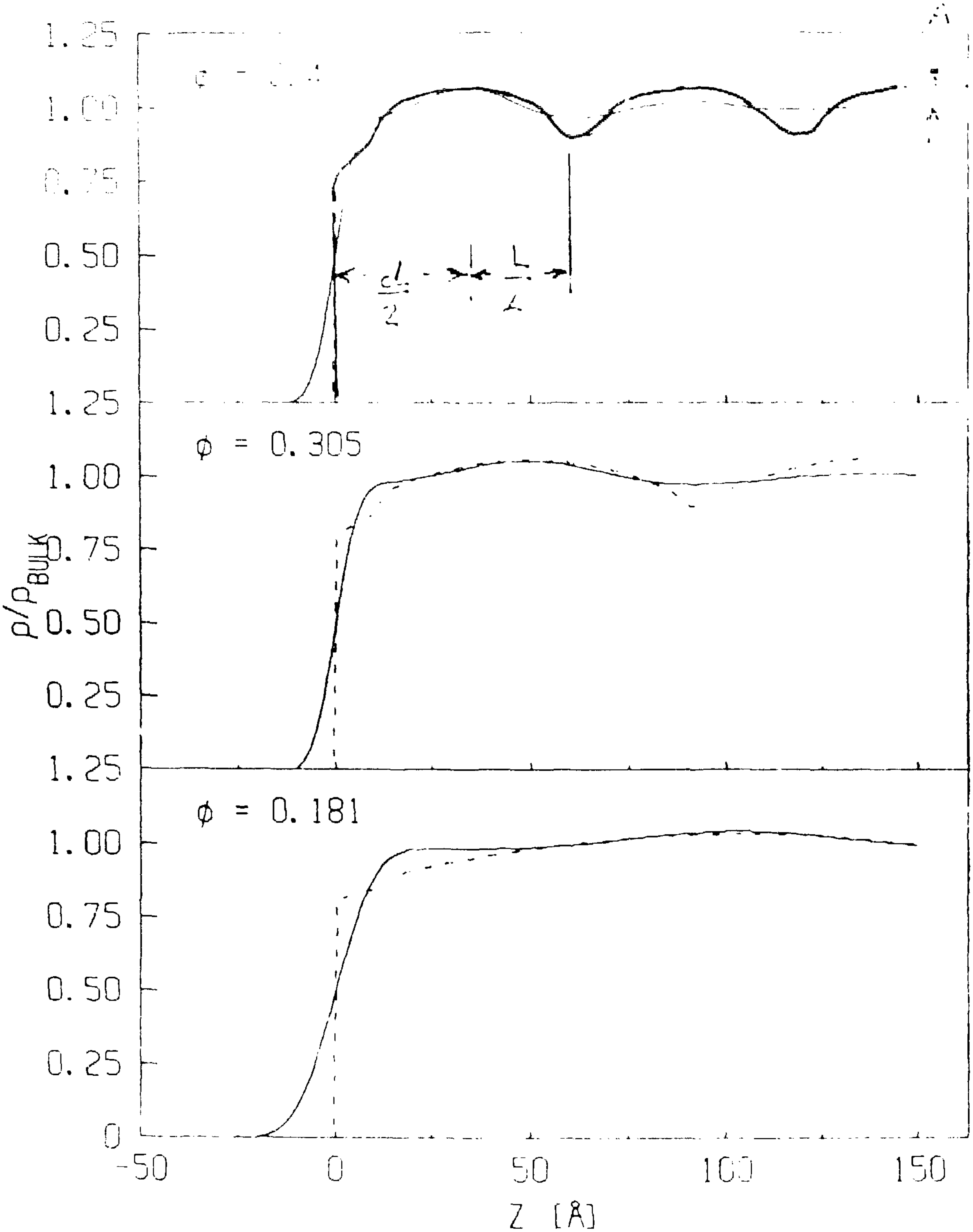
REPRODUCED FROM BEST
AVAILABLE COPY



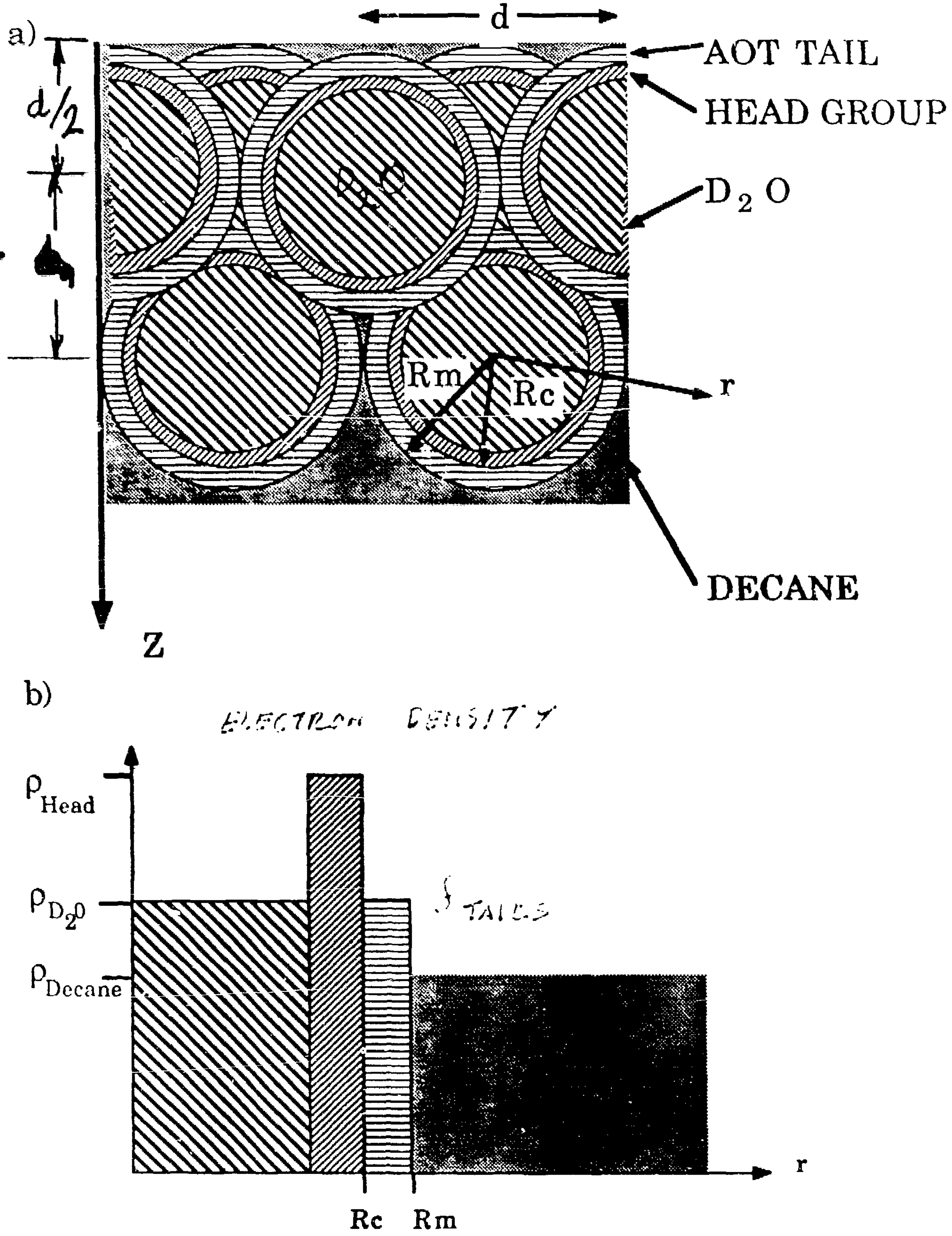
Ocko
Tidswell




AOT 0.42
DAM SCHWARTZ
Φ=0.42
R/R_f
10
1
0.1
0
0.05
0.10
0.15
0.20
0.25
q_z [Å^-1]



ϕ = 0.305
ϕ = 0.181
ρ/ρ_BULK
1.25
1.00
0.75
0.50
0.25
0
-50
0
50
100
150
Z [Å]
d/2
L/2



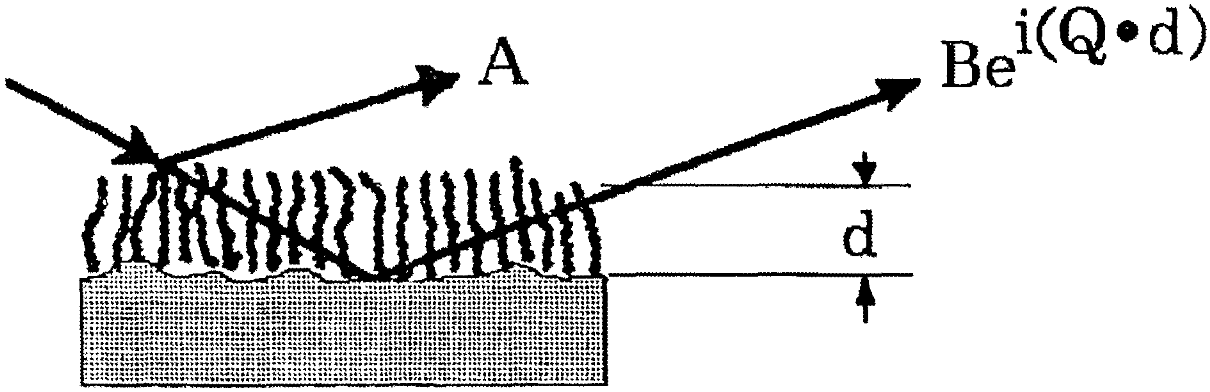
a)
d
AOT TAIL
HEAD GROUP
d/2
D_2O
L
Rm
Rc
r
DECANE
Z
b)
ELECTRON DENSITY
ρ_{Head}
ρ_{D_2O}
TAILS
ρ_{Decane}
r
Rc
Rm

HYROCARBON COATED SiO_2/Si

with George Whitesides

Self Assembling Monolayers:

C_n-Silanes(n=10 ~ 22)



Density of Si≈Density of SiO_2

Density of $(-CH_2-)_n \approx 0.43$ Density of Si

Without Roughness: $A \propto 0.43$

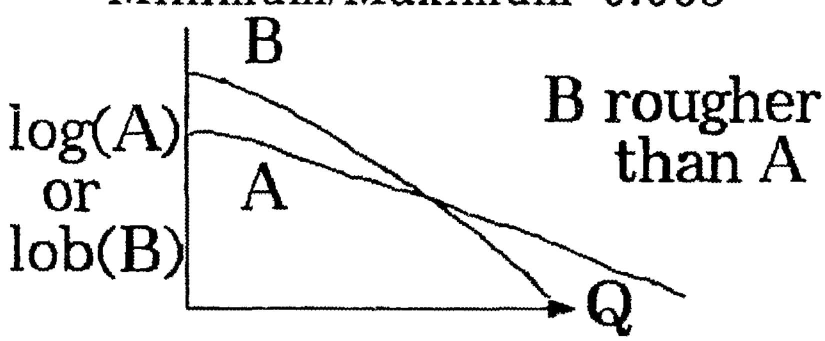
$B \propto (1-0.43)$

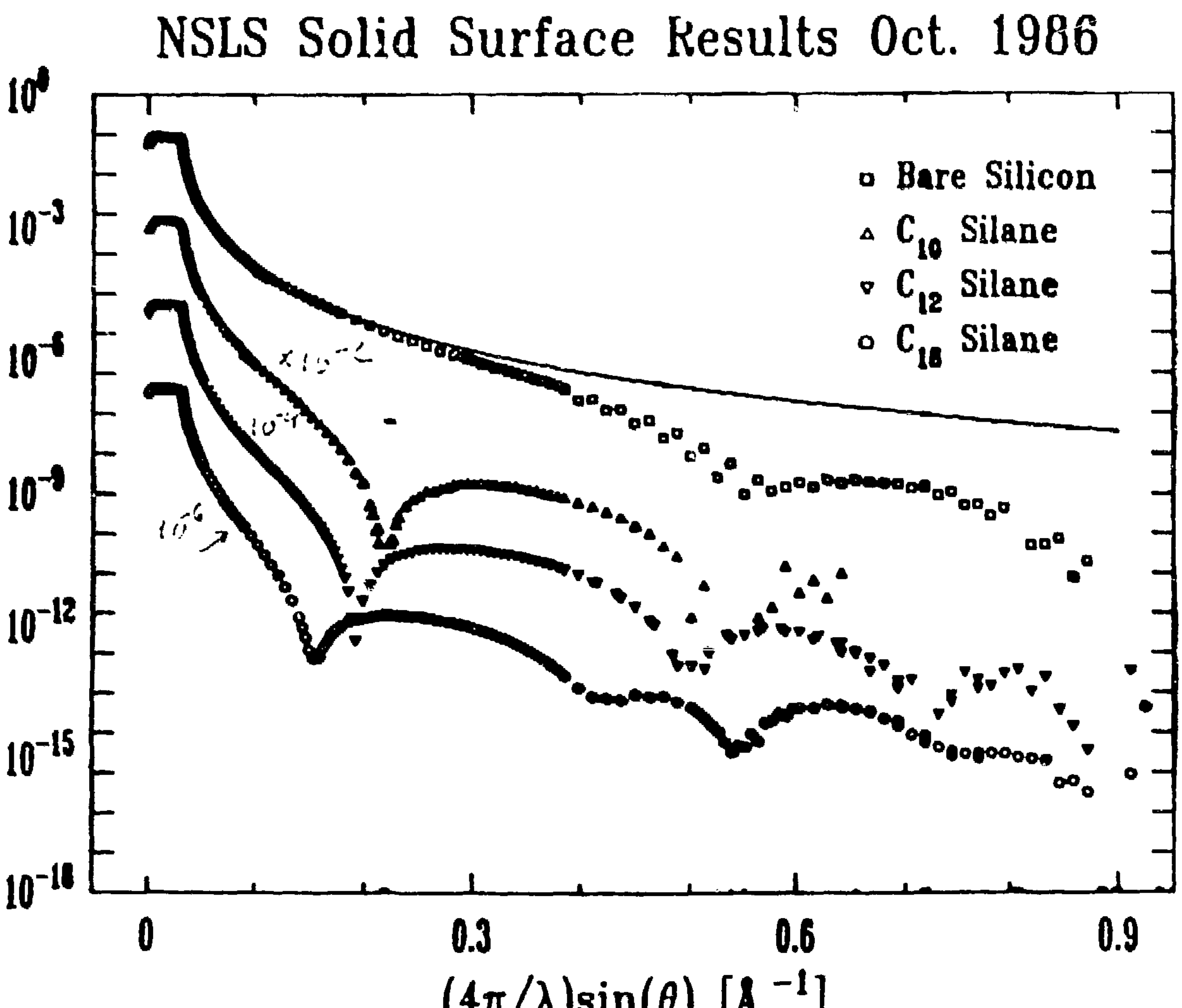
$\text{Minimum} \approx (A-B)^2 \approx (1-0.86)^2 \approx 0.02$

$\text{Maximum} \approx (A+B)^2 \approx 1.0$

Observed

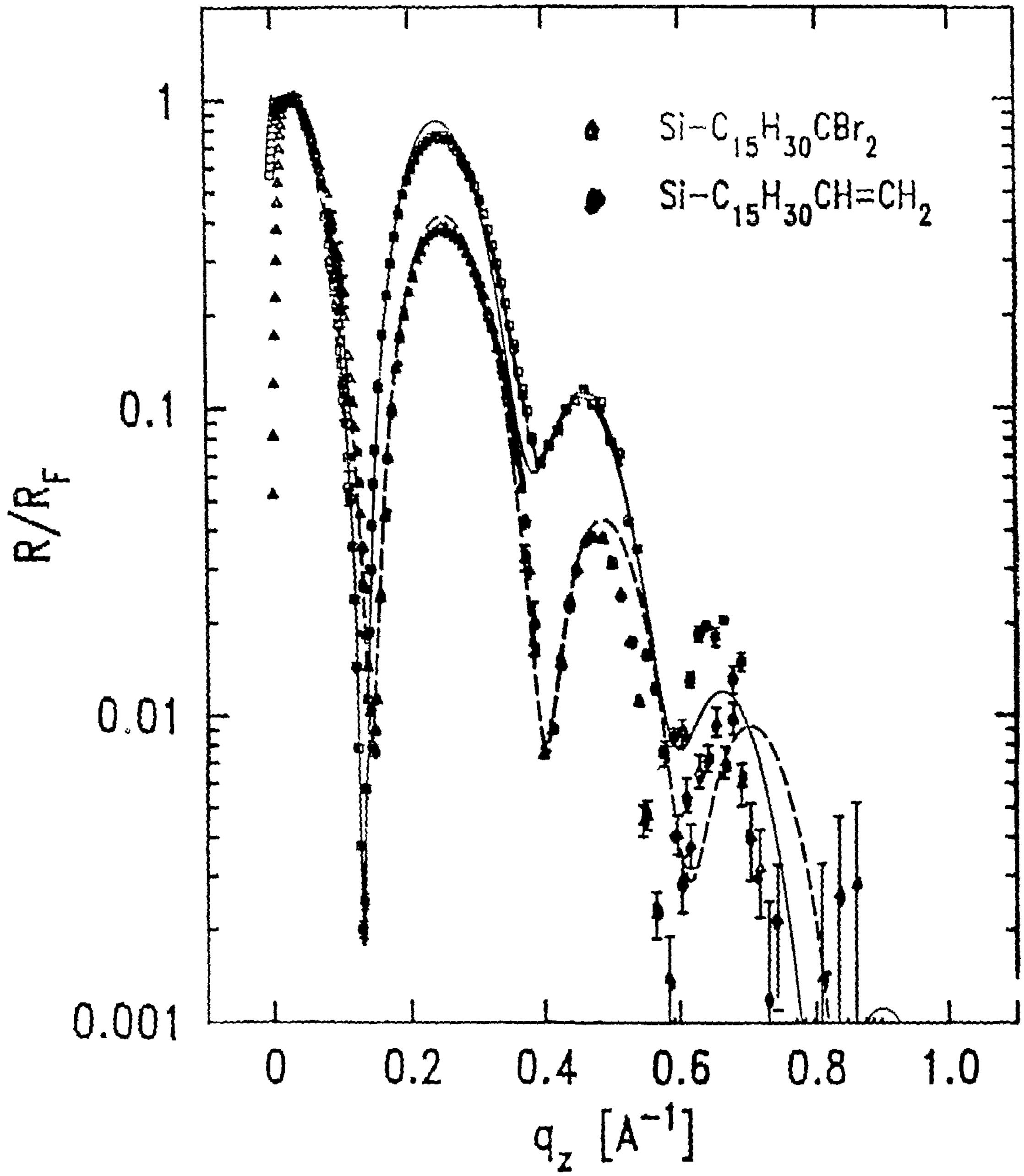
Minimum/Maximum≈0.008





NSLS Solid Surface Results Oct. 1986
Bare Silicon
C10 Silane
C12 Silane
C18 Silane
10^0
10^-3
10^-6
10^-9
10^-12
10^-15
10^-18
0
0.3
0.6
0.9
(4π/λ)sin(θ) [Å^-1]

Double Bond Termination and Bromination

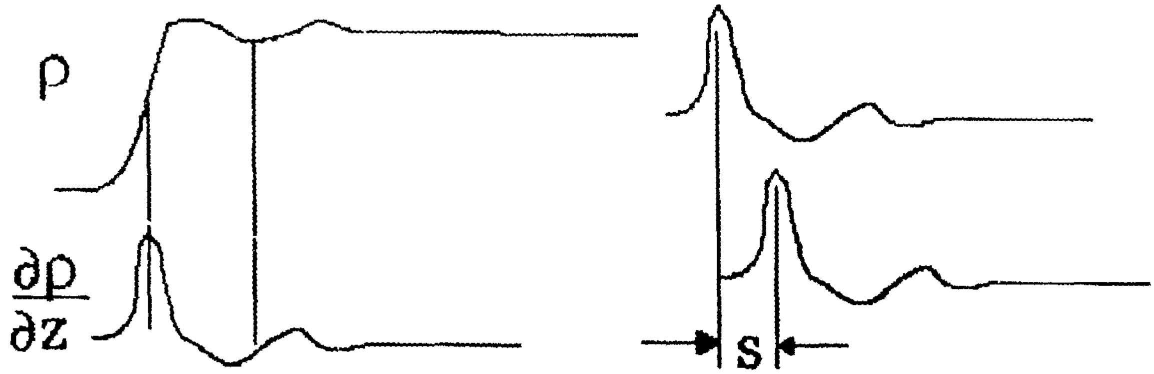


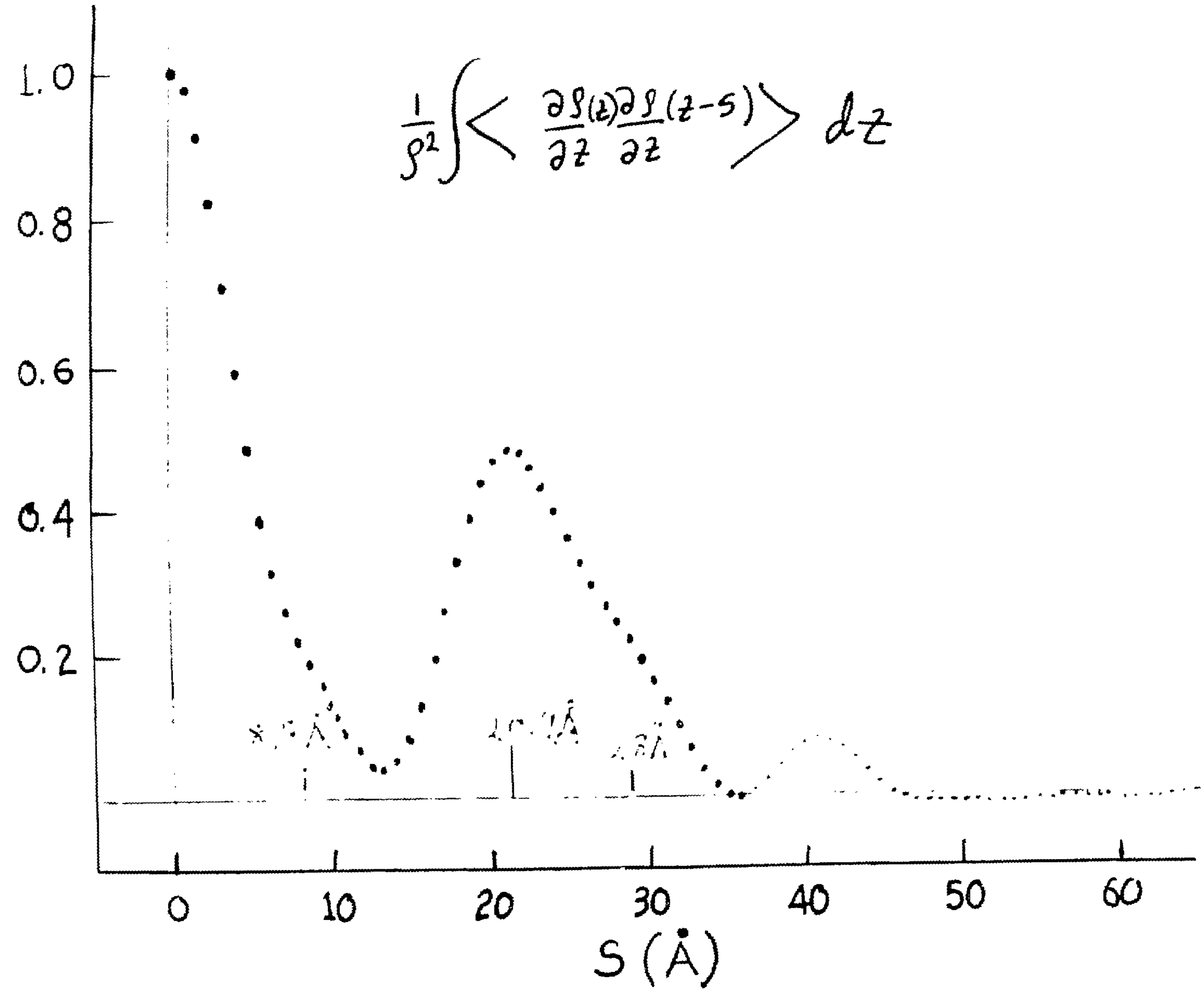
PATTERSON FUNCTION

$$\frac{R(\theta)}{R_F(\theta)} = \left| \frac{1}{\rho_\infty} \int dz \left\langle \frac{\partial \rho}{\partial z} \right\rangle e^{i(Q \bullet z)} \right|^2$$

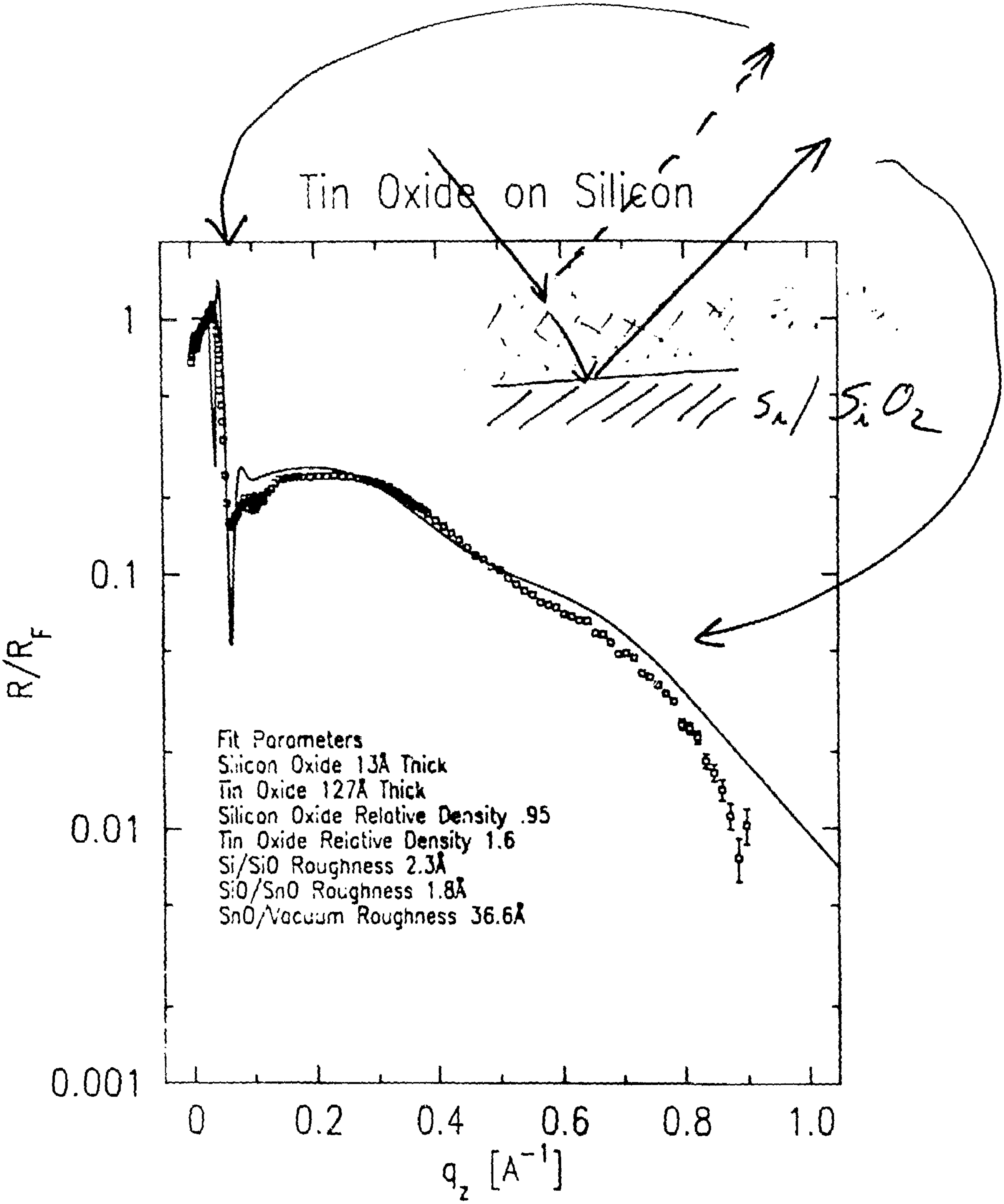
$Q=(4\pi/\lambda)\sin(\theta)$

$$\int \frac{1}{\rho^2} \left\langle \frac{\partial \rho}{\partial z} \frac{\partial \rho(s-z)}{\partial(s-z)} \right\rangle dz = \frac{1}{2\pi} \int dQ e^{iQ \bullet s} \left\{ \frac{R(Q)}{R_F(Q)} \right\}$$



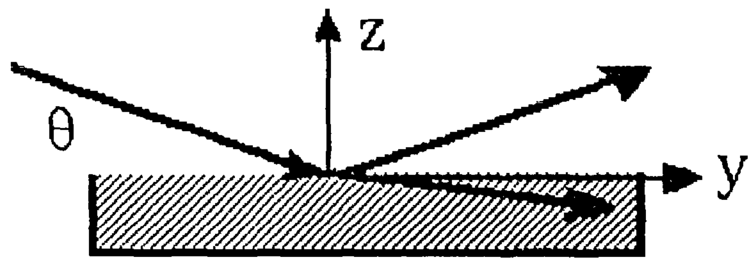


$\frac{1}{\rho^2}\int\left\langle \frac{\partial\rho(z)}{\partial z}\frac{\partial\rho}{\partial z}(z-s)\right\rangle dz$
1.0
0.8
0.6
0.4
0.2
0
10
20
30
40
50
60
S (Å)


Tin Oxide on Silicon
Si/SiO2
1
0.1
0.01
0.001
R/R_F
Fit Parameters
Silicon Oxide 13Å Thick
Tin Oxide 127Å Thick
Silicon Oxide Relative Density .95
Tin Oxide Relative Density 1.6
Si/SiO Roughness 2.3Å
SiO/SnO Roughness 1.8Å
SnO/Vacuum Roughness 36.6Å
0
0.2
0.4
0.6
0.8
1.0
q_z [A^-1]

THEORY FOR DIFFUSE (ROUGH) SURFACE

$$\nabla^2 E + \varepsilon(z) k_0 E = 0$$



$$E = e^{i(k_y y)} \psi(z)$$

$$-\partial^2\psi/\partial z^2 + [k_y^2 - \varepsilon(z) k_0^2]\,\psi = 0$$

$$-\partial^2\psi/\partial z^2 + k_o^2[\cos^2(\theta) - \varepsilon(z)\}]\psi = 0$$

$$\boxed{-\partial^2\psi/\partial z^2 + k_o^2[-\theta^2 + \theta_c^2]\psi = 0}$$

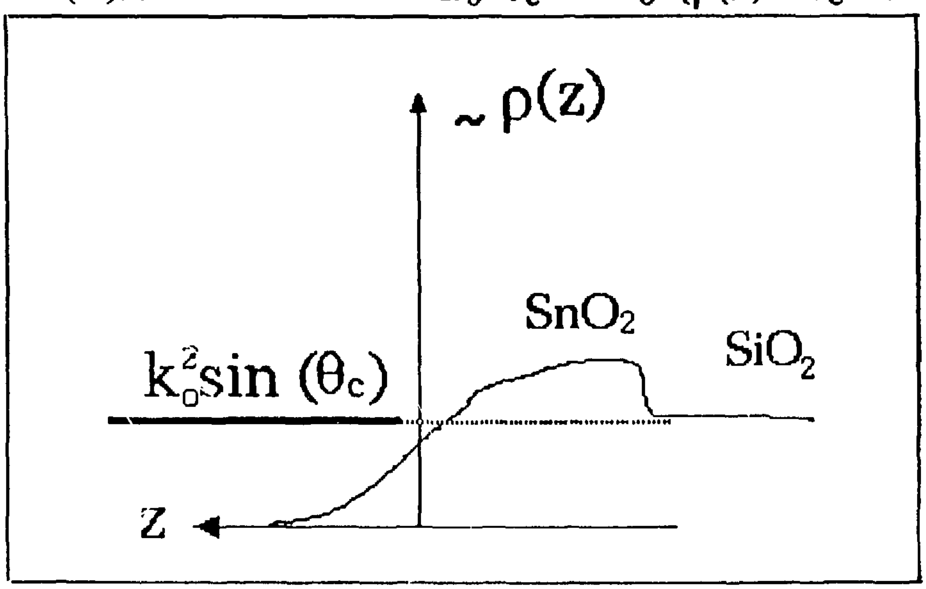
Electron Motion in One Dimension

$$p^2/2m + V(z) = p_0^2/2m$$

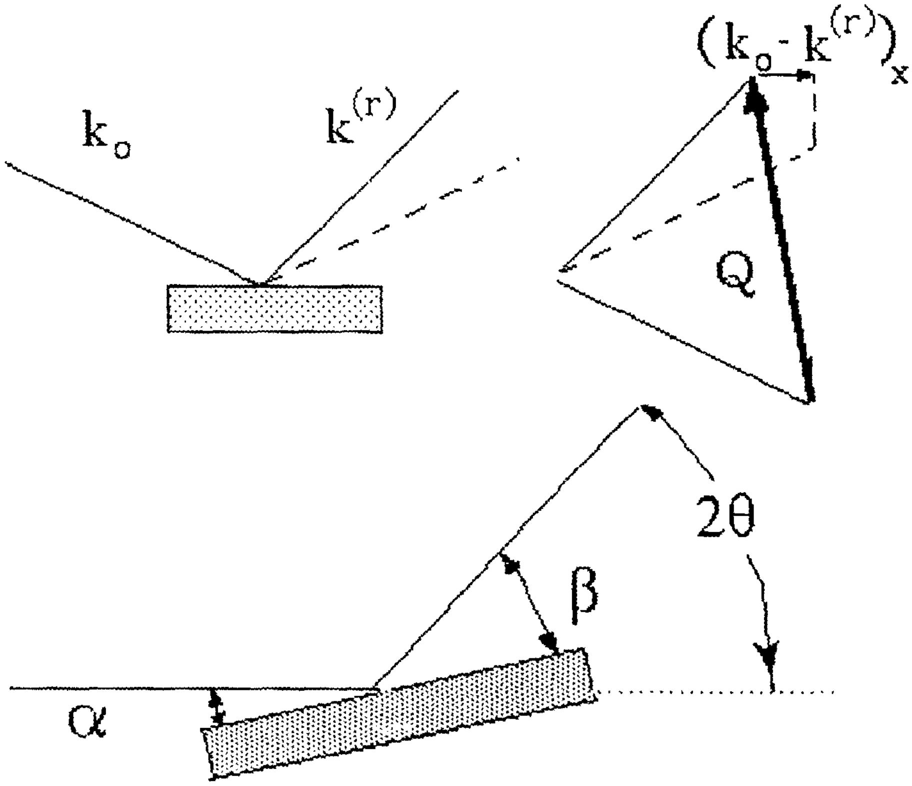
$$-[\hbar^2/2m]\partial^2\psi/\partial z^2 + [-p_0^2/2m + V(z)]\psi = 0$$

ANALOGY

$p_0^2/\hbar^2$	$\Rightarrow$	$k_0^2\theta^2$
$2mV(z)/\hbar^2$	$\Rightarrow$	$k_0^2\theta_c^2 \approx k_0^2\{\rho(z)e^2 r_e \lambda^2/\pi\}$



DIFFUSE SCATTERING



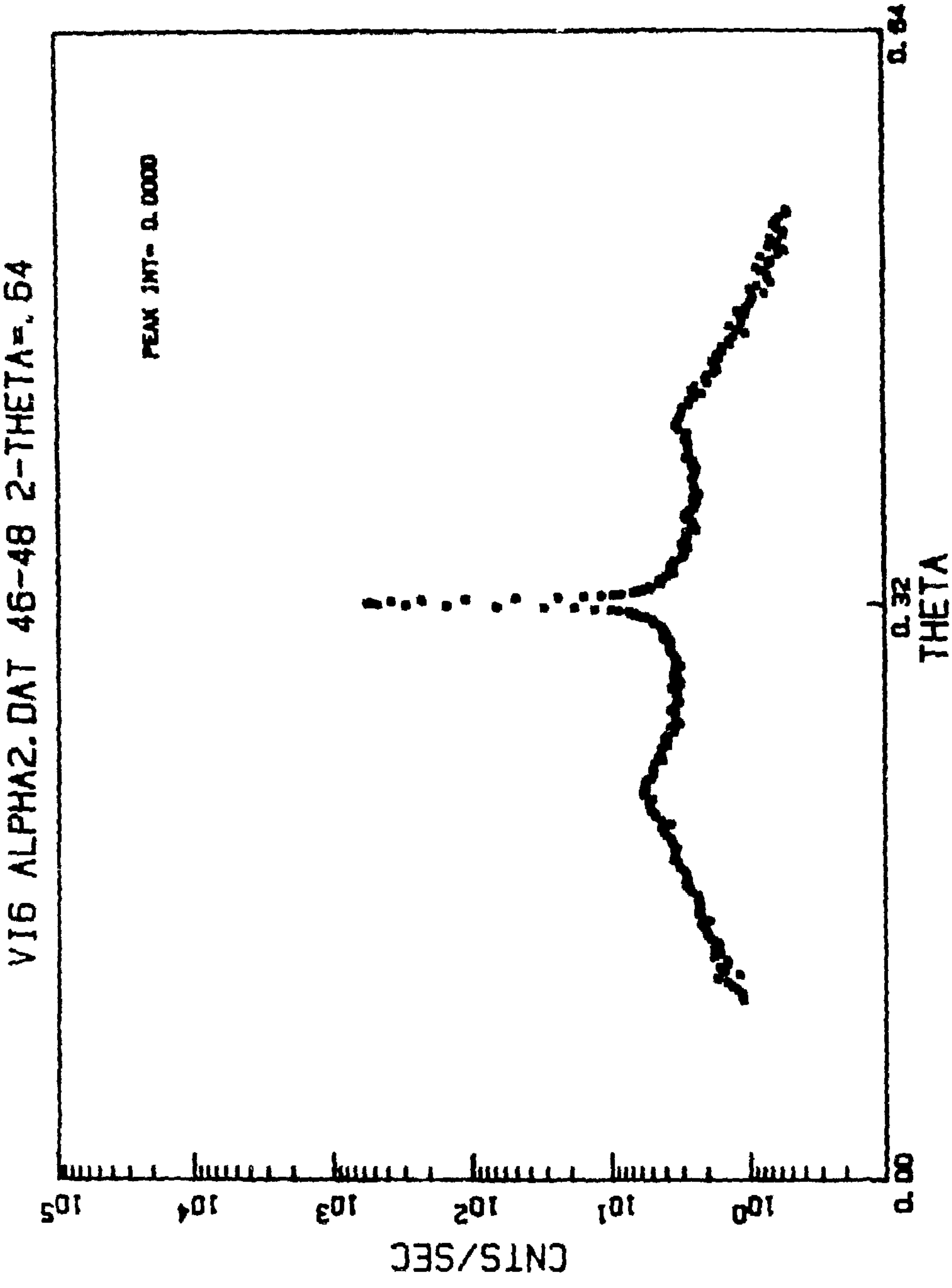
$$\frac{d\sigma}{d\Omega} = \frac{\sqrt{R_F(\alpha)R_F(\beta)}}{(4\pi)^2}(QQ')^2\left(\frac{S_o}{\alpha}\right)\int d\mathbf{x} \langle h(0)h(\mathbf{x})\rangle e^{i(\mathbf{k}^{(r)}-\mathbf{k}_o)\bullet\mathbf{x}}$$

$$Q^2\sqrt{R_F(\alpha)} \approx \frac{4\alpha^2}{\left(\alpha+\sqrt{\alpha^2-\theta_c{}^2}\right)^2}$$

$$\approx 4 \text{ for } [\alpha \approx \theta_c]$$

$$\approx 1 \text{ for } [\alpha < \theta_c]$$

$$\approx \left(\frac{\alpha}{2\theta_c}\right)^2 \text{ for } [\alpha >> \theta_c]$$


VIG ALPHA2.DAT 46-48 2-THETA=.64
PEAK INT= 0.0000
CNTS/SEC
0
10^0
10^1
10^2
10^3
10^4
10^5
0.00
0.32
0.64
THETA

SUMMARY

TO DATE: Rotating Anode & Bending Magnet Radiation

SPECULAR REFLECTIVITY OF LIQUID SURFACES:

1 - Simple Liquids	Roughness
2 - Liquid Crystal	Induced Layered Structure
3 - Micelles	Nature of Surface

SOLID SURFACES

1 - Silane Coated Si/SiO_2	Thickness Uniformity Structure
2 - SnO_2	Buried Surface
3 - Glasses	Surface Specific Diffuse Scattering

WORK BY OTHERS

1 - In Plane Structure of Monolayers on H_2O
Als-Nielsen, et al. Phys. Rev. Lett. **58**, 2224(1986)
Dutta, Rice, et al. Preprint (1986)

2 - Liquid Metals
Rice, Nature, **316**, 108(1986)
Bosio, J. Chem. Phys., **80**, 959(1984)

POSSIBILITIES FOR FUTURE: Wiggler Lines, etc.

1 - Solids Samples Smaller than Incident Beam
2 - Liquid/Solid Interface
3 - Small Angle Diffuse Scattering From Liquid Surfaces
Bonse-Hart Crystal Analyzer

TIME-RESOLVED MACROMOLECULAR CRYSTALLOGRAPHY*

Keith Moffat
Cornell University

ABSTRACT

The essential link between macromolecular structure at the atomic level and biochemical function has proved remarkably difficult to establish. Although several hundred such structures have now been determined through the efforts of numerous x-ray crystallographers, the number of well-established mechanisms of action is a great deal smaller. Even for those mechanisms that are apparently understood, new insights provided by protein engineering have often revealed the limitations on our understanding.

Why is the structural basis of mechanism so difficult to establish? I believe that this is due, in large part, to the inability of classical x-ray crystallography to examine short-lived structures, such as catalytic intermediates, or intermediates in ligand binding and release, or in the early stages of protein unfolding. Many macromolecules are active in the crystal, and hence structural intermediates do exist and may be accessible to, for example, spectroscopic probes. Can they be made accessible to crystallographic probes that will reveal the transient changes in atomic structure directly? Here, the goal is to develop time-resolved macromolecular crystallography: the technique itself, and the biochemical systems to which it may be applied.

Time-resolved crystallography is based on three main areas. The best time resolution is accessible with the highest incident x-ray intensity, which depends on the x-ray source (for example, undulator vs. wiggler vs. bending-magnet sources at the Cornell High Energy Synchrotron Source, CHESS, or the Advanced Photon Source, APS), on the x-ray optics (for example, focusing vs. nonfocusing), and on the x-ray technique (for example, polychromatic Laue vs. monochromatic). Second, techniques for uniform, rapid reaction initiation throughout the crystal, such as laser photolysis, pose a major experimental challenge. And third, data acquisition and reduction with the necessary integrating detectors (for example, film or the Kodak storage phosphor detector) is not straightforward.

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*The following abstract and copies of viewgraphs were provided by the speaker.

The principles of time-resolved macromolecular crystallography will be discussed and illustrated with examples of preliminary studies at CHESS and Daresbury.

K.M. 27/1/86

"THAT'S NO GOOD! CRYSTALS DON'T WRIGGLE, AND IF IT DOESN'T WRIGGLE, IT'S NOT BIOLOGY"

THE PHYSIOLOGIST A.V. HILL, COMMENTING ON JOHN KENDREW'S PLANS TO STUDY PROTEIN CRYSTALS

(c. 1948)

WHY TIME - RESOLVED CRYSTALLOGRAPHY?

"MECHANISM" INVOLVES <u>CHANGES</u> IN STRUCTURE

e.g. CATALYSIS BY ENZYMES;

LIGAND BINDING BY HEME PROTEINS, OR

CALCIUM BINDING PROTEINS, OR IMMUNOGLOBULINS;

MUSCLE CONTRACTION; PROTEIN UNFOLDING;

TUBULIN POLYMERIZATION;

THESE MAY BE VERY RAPID, << 1S

CAN CHANGES IN STRUCTURE BE INITIATED, RAPIDLY AND UNIFORMLY, IN THE CRYSTAL?

CAN SUBSEQUENT CHANGES IN STRUCTURE AMPLITUDES BE MONITORED IN REAL TIME, AND ANALYZED?

— POPULATIONS; LIFETIMES; ISOMORPHISM

WHY USE LAUE DIFFRACTION?

- <u>FASTEST</u> i.e. SHORTEST POSSIBLE EXPOSURES
- MOST <u>EFFICIENT</u> i.e. FEW EXPOSURES PER DATA SET
- INTEGRATED INTENSITIES FROM A <u>STATIONARY</u> CRYSTAL
- CAN BE PRECISELY <u>QUANTITATED</u>, DESPITE THE <u>APPARENT</u> "OVERLAPPING ORDERS PROBLEM".

METHODS OF REACTION INITIATION

1) FLOW CELL

EFFECTIVE ONLY WHEN REACTIONS ARE SLOWER THAN DIFFUSION RATES

i.e. $t_{\frac{1}{2}} \gtrsim 150$ s

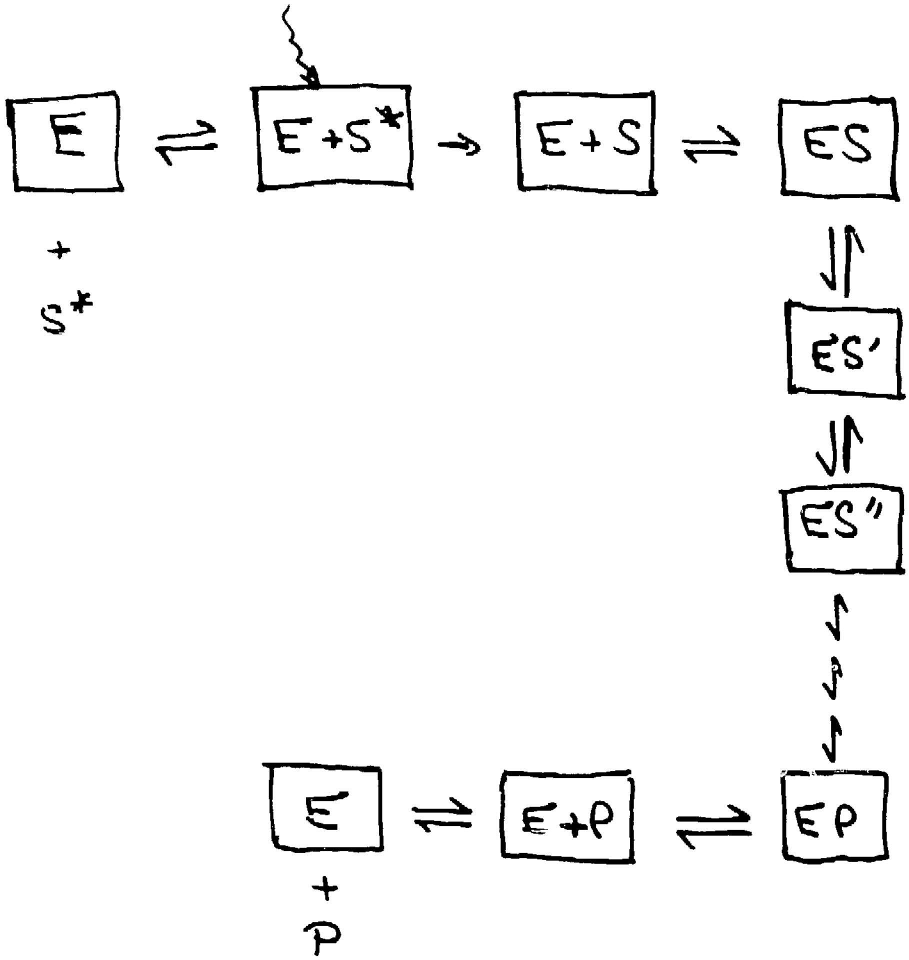
2) PHOTOACTIVATION

- NATURAL e.g. CO-HEMOGLOBIN, CO-MYOGLOBIN, PHOTOSYNTHETIC REACTION CENTERS
- SYNTHETIC e.g. CAGED SUBSTRATES, CAGED PROTONS

3) CHANGE IN A PHYSICAL PARAMETER

- TEMPERATURE
- PRESSURE

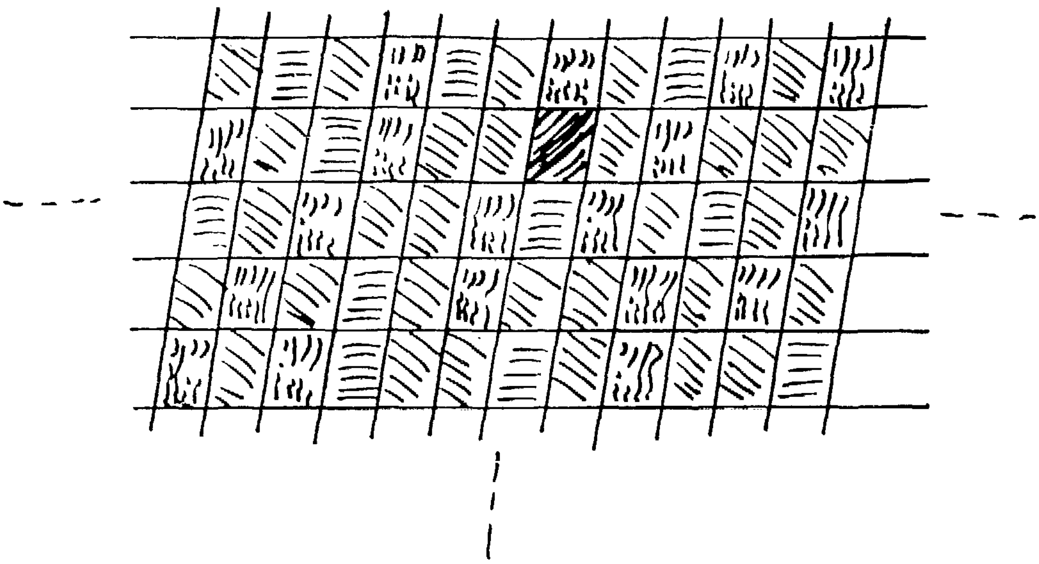
REACTIONS MAY BE IRREVERSIBLE i.e. SINGLE SHOT OR REVERSIBLE ∴ MULTIPLE SHOTS ARE POSSIBLE, TO ENHANCE SIGNAL-TO-NOISE OR TO LOWER THE TIME RESOLUTION. STROBOSCOPIC EXPERIMENTS CAN BE ENVISAGED e.g. nS RE-ANNEALING OF Si SINGLE CRYSTALS AFTER LASER-INDUCED MELTING. ULTIMATE TIME RESOLUTION SET BY THE X-RAY PULSE LENGTH, 150 ps AT CHESS.



$S^* \rightarrow S +$ "CAGE"

VIA REACTIVE INTERMEDIATES
WHICH ARE SHORT-LIVED, USUALLY $\lesssim$ ms ;
CAGE MAY BE REACTIVE.

DO THESE SIDE REACTIONS INTERFERE?



FIVE CONFORMATIONS :

EACH CONFORMATION IS DESCRIBED AS THE CONVOLUTION OF THAT STRUCTURE WITH A RANDOMLY SPARSE LATTICE ; THE REAL CRYSTAL IS THEN THE SUM OF FIVE SUCH CONVOLUTIONS .

DIFFRACTION FROM THE CRYSTAL IS THEN THE SUM OF EACH MOLECULAR TRANSFORM × THE RECIPROCAL (SPARSE) LATTICE ASSOCIATED WITH IT .

THE TRANSFORM OF A RANDOMLY SPARSE REAL LATTICE IS A RECIPROCAL LATTICE WHERE EACH POINT IS WEIGHTED BY THE FRACTION OF POINTS OCCUPIED IN THE REAL LATTICE .

THE ABOVE ASSUMES THAT ISOMORPHISM OF THE CRYSTAL LATTICE IS MAINTAINED .

KM 11/7/86

IF AT ANY INSTANT A CRYSTAL CONTAINS A SERIES OF CONFORMATIONS C1, C2, C3 ... Ci ..., DISTRIBUTED AT RANDOM, WITH FRACTIONAL OCCUPANCIES f_{ci} AND STRUCTURE FACTORS $\underline{F}_{ci}(\underline{h})$ FOR THE REFLECTION $\underline{h}$, THEN THE TOTAL STRUCTURE FACTOR $\underline{F}(\underline{h}, t)$ IS GIVEN BY

$$\underline{F}(\underline{h}, t) = \sum_i f_{ci}(t)\, \underline{F}_{ci}(\underline{h})$$

AND

$$\sum_i f_{ci}(t) = 1$$

FOR ALL TIMES t.

THAT IS, THE FRACTIONAL OCCUPANCIES VARY IN TIME; THE INDIVIDUAL STRUCTURE FACTORS DO NOT.

NOTE THAT THIS IS A VECTOR SUM; THE PHASES OF EACH OF THE $\underline{F}_{ci}(\underline{h})$ VARY WITH i. IF THE Ci ARE CLOSELY SIMILAR IN STRUCTURE, THE DIFFERENCES IN PHASE WILL BE SMALL.

THE FUNCTIONAL FORM OF THE TIME DEPENDENCE OF EACH REFLECTION IS THE SAME; ALL REFLECTIONS TOGETHER MAY BE USED TO OBTAIN THIS FORM.

IN GENERAL, THIS FUNCTIONAL FORM IS A SUM OF EXPONENTIALS. THAT IS,

$$\underline{F}(\underline{k},t) = \sum_{j=1}^{N} \underline{A}_j(\underline{k}) \exp[-k_j t]$$

WHERE k_j ARE FIRST ORDER RATE CONSTANTS AND $\underline{A}_j(\underline{k})$ ARE A FUNCTION OF ALL THE k_j AND ALL THE $\underline{F}_{ci}(\underline{k})$.

NOW $\Delta F_L(\underline{k},\lambda,t)/F_L(\underline{k},\lambda,0)$

$$= \{|\underline{F}(\underline{k},t)| - |\underline{F}(\underline{k},0)|\} / |\underline{F}(\underline{k},0)| .$$

IF NOW $f_{c1}(0) = 1$ AND $f_{ci}(0) = 0$ FOR $i \neq 1$, THEN

$$\Delta F_L(\underline{k},\lambda,t)/F_L(\underline{k},\lambda,0)$$
$$= \{|\sum_{j=1}^{N} \underline{A}_j(\underline{k}) \exp[-k_j t]| - |\underline{F}_{c1}(\underline{k})|\} / |\underline{F}_{c1}(\underline{k})|$$

– ONLY RELATIVE CHANGES IN (LAUE) INTENSITIES ARE NEEDED, A MAJOR SIMPLIFICATION.

AS AN EXAMPLE, CONSIDER CONSECUTIVE IRREVERSIBLE REACTIONS

$$\begin{array}{ccccc} E & \xrightarrow{k_1} & E' & \xrightarrow{k_2} & E'' \\ c1 & & c2 & & c3 \end{array}$$

ASSUME $f_{c_1}(0) = 1, \; f_{c_2}(0) = f_{c_3}(0) = 0$.

THEN

$$f_{c_1}(t) = \exp[-k_1 t]$$

$$f_{c_2}(t) = \{k_1/(k_2-k_1)\}\{\exp[-k_1 t] - \exp[-k_2 t]\}$$

$$f_{c_3}(t) = 1 - \{f_{c_1}(t) + f_{c_2}(t)\}$$

$$= 1 + \{k_2 \exp[-k_1 t] - k_1 \exp[-k_2 t]\}/\{k_1 - k_2\} .$$

THUS $\underline{F}(\underline{h}, t) = \sum_{i=1}^{3} f_{ci}(t)\, \underline{F}_{ci}(\underline{h})$

$$= \left\{\underline{F}_{c_1}(\underline{h}) + \frac{k_1}{k_2-k_1}\underline{F}_{c_2}(\underline{h}) + \frac{k_2}{k_1-k_2}\underline{F}_{c_3}(\underline{h})\right\} \times \exp[-k_1 t]$$

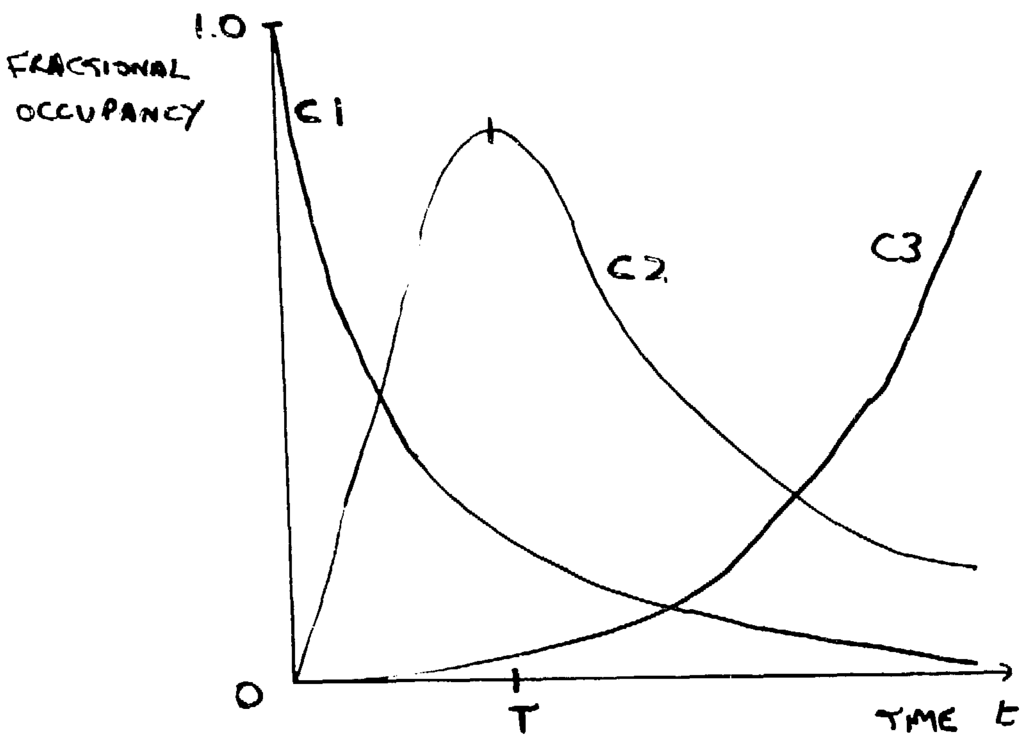
$$+ \left\{\frac{k_1 \underline{F}_{c_2}(\underline{h})}{k_1 - k_2} + \frac{k_1 \underline{F}_{c_3}(\underline{h})}{k_2 - k_1}\right\} \exp[-k_2 t]$$

$$+ \{\underline{F}_{c_3}(\underline{h})\}.$$

EACH TERM { } IS A COEFFICIENT $\underline{A}_j(\underline{h})$, WHICH IS CONSTANT IN TIME AND PHASE

THIS IS A DOUBLE EXPONENTIAL, A CLEAR INDICATION THAT THERE IS (AT LEAST) ONE INTERMEDIATE CONFORMATION, HERE DENOTED E' (C2).

TO DETECT IT, IT MUST ATTAIN A MEASURABLE CONCENTRATION AND HAVE A LIFETIME GREATER THAN THE X-RAY TIME RESOLUTION.



T, THE TIME AT WHICH MAXIMUM OCCUPANCY OF C2 IS ATTAINED, IS GIVEN BY

$$T = (k_1 - k_2)^{-1} \ln (k_1/k_2) .$$

FOR THE INTERMEDIATE TO ACCUMULATE, $k_1 > k_2$ AND AT $t = T$, THEN THE FRACTIONAL OCCUPANCY OF C2 IS

$$f_{C2}(T) = \{k_1/(k_2 - k_1)\}\{\exp[-k_1 T] - \exp[-k_2 T]\}.$$

NOW $f_{C2}(T)$ DEPENDS ONLY ON k_1/k_2, AND TENDS TO $1/e = 0.3678$ AS $k_1 \to k_2$.

k_1 s^{-1}	k_2 s^{-1}	T s	$f_{C2}(T)$
50	10	.0402	.669
5	1	.402	.669
2	1	.693	.500
1.5	1	.811	.444
1.1	1	.953	.385
1.01	1	.995	.370
1	1	1	.3678...

THUS, IN THIS EXAMPLE EVEN THE LOWEST CONCENTRATION SHOULD BE DETECTABLE, OF AN ACCUMULATING INTERMEDIATE. PROVIDED ALSO THAT THE TOTAL TIME FOR WHICH $f_{C2}(t) > 0.35$ (SAY) IS GREATER THAN ~ 5× THE X-RAY EXPOSURE. THIS DEPENDS ON THE MAGNITUDES OF THE RATE CONSTANTS, NOT JUST ON THEIR RATIO.

WHAT IS THE TIME RESOLUTION IN A SINGLE CRYSTAL LAUE DIFFRACTION EXPERIMENT ?

THIS DEPENDS ON:

1) THE INTENSITY FALLING ON THE CRYSTAL
2) THE SCATTERING POWER OF THE CRYSTAL
3) THE LIKELY MAGNITUDE OF THE INTENSITY CHANGES, AND HENCE THE PRECISION WITH WHICH THEY MUST BE MEASURED
4) THE DETECTOR SENSITIVITY, NOISE CHARACTERISTICS AND RESPONSE TIME.

CONSIDER 1) AND 2) THE INTEGRATED INTENSITY E_L FOR A LAUE REFLECTION OF STRUCTURE AMPLITUDE $|F|$ IN AN EXPOSURE TIME Δt IS

$$E_L / |F|^2 \Delta t = \gamma_e I'(\lambda) \lambda^4 \frac{V}{V_0^2} (2\sin^2\theta)^{-1} . i . (kRPA/D_F)$$

PHOTONS s^{-1} cm^{-2}

WHERE γ_e = (RADIUS OF THE ELECTRON)^2 ; λ = WAVELENGTH OF THE REFLECTION

V = CRYSTAL VOLUME ILLUMINATED ; V_0 = UNIT CELL VOLUME

θ = BRAGG ANGLE ; i = SYNCHROTRON CURRENT

$I'(\lambda)$ = SOURCE SPECTRAL INTENSITY DISTRIBUTION

R = REFLECTIVITY OF OPTICS ; P = POLARIZATION FACTOR OF OPTICS

A = mrad ACCEPTED BY OPTICS

D = FOCAL SPOT SIZE

CONSIDER 3). ASSUME $\langle \Delta I / I \rangle \sim 10\%$. THEN, WE MUST MEASURE INTENSITIES TO WITHIN A PRECISION OF, SAY, 2%, OR MORE GENERALLY $p\%$.

FOR A PERFECT DETECTOR, THIS REQUIRES $10^4/p^2$ PHOTONS WHERE p IS IN %.

ASSUME THAT FOR A REAL DETECTOR AT WAVELENGTH λ, THIS REQUIRES $10^4 K^2/p^2$ PHOTONS WHERE $K > 1$.

ALSO ASSUME THAT THE RESPONSE TIME OF THE DETECTOR IS NOT RATE-CONTRIBUTING.

THEN THE EXPOSURE TIME Δt THAT WILL YIELD A PRECISION $p\%$ FOR A REFLECTION $|F|$ IS

$$\Delta t = \frac{10^4 K^2 V_0^2 \cdot 2\sin^2\theta}{j_e \lambda^4 V_i \left(l I' R \mu A / D_F \right) |F|^2 p^2}$$

FOR NON-CENTROSYMMETRIC STRUCTURES, THE MEDIAN STRUCTURE AMPLITUDE IS $0.832\sqrt{\langle I \rangle}$. FOR PROTEINS, $\langle I \rangle \approx 3.2\, Mn$ WHERE M IS THE MOLECULAR WEIGHT AND n IS THE NUMBER OF MOLECULES PER UNIT CELL.

HENCE THE MEDIAN $|F|^2$ IS $2.2\, Mn\ \ e^2$

FOR A PRESENT-DAY CHESS BENDING MAGNET

AT 1 Å ; 12 m FROM SOURCE ; 200 μm APERTURE ;

NO FOCUSSING ; 30 mA

THEN $E_L / |F|^2 \Delta t = 2.4 \times 10^{-40} \dfrac{V}{V_0^2 \sin^2 2\theta}$

WHERE V , THE VOLUME ILLUMINATED,

AND V_0 , THE UNIT CELL VOLUME,

ARE IN m^3 .

E.G. MYOGLOBIN $V_0^2 = 4.38 \times 10^{-51}$ m^6

$V = (200\ \mu m)^3 = 8 \times 10^{-12}$ m^3

AT $\theta = 15^\circ$,

$E_L / |F|^2 \Delta t = 6.4$ PHOTONS s^{-1} EL^{-2}

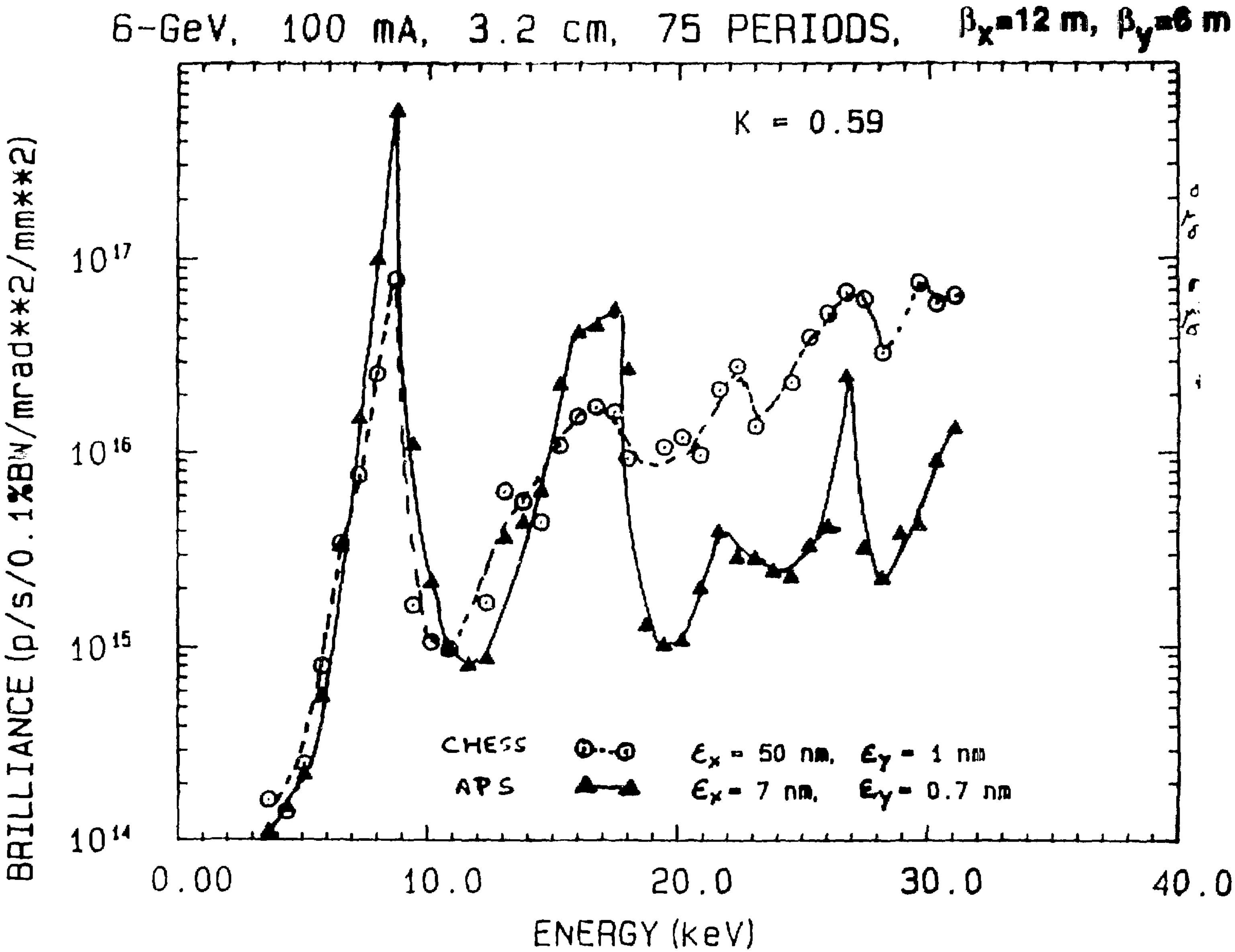
THE MEDIAN $|F|$ IS 270 ELECTRONS

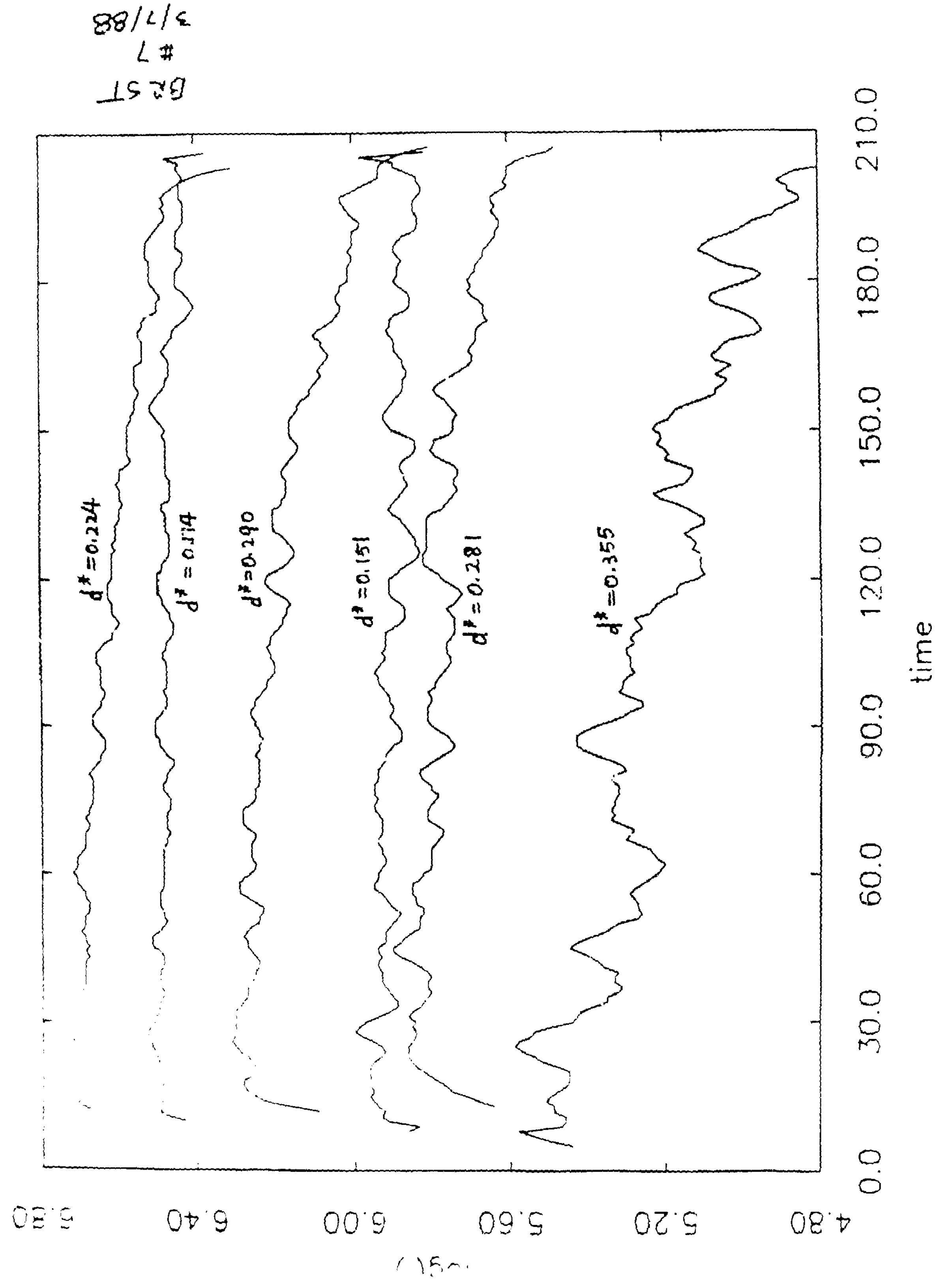
∴ THE MEDIAN $E_L / \Delta t$ IS 4.7×10^5 PHOTONS s^{-1}

∴ 10^4 PHOTONS ARE DIFFRACTED INTO A REFLECTION OF MEDIAN INTEGRATED INTENSITY IN 21 ms

THE FLUX FALLING ON THE CRYSTAL, IN A 20% BANDPASS, THROUGH A 200 μm APERTURE, IS ROUGHLY

5×10^{11} PHOTONS s^{-1}


6-GeV, 100 mA, 3.2 cm, 75 PERIODS, βx=12 m, βy=6 m
K = 0.59
BRILLIANCE (p/s/0.1%BW/mrad**2/mm**2)
10^17
10^16
10^15
10^14
0.00
10.0
20.0
30.0
40.0
ENERGY (keV)
CHESS
APS
εx = 50 nm, εy = 1 nm
εx = 7 nm, εy = 0.7 nm



B2 5T
7
3/7/88
$d^*=0.224$
$d^*=0.114$
$d^*=0.290$
$d^*=0.151$
$d^*=0.281$
$d^*=0.355$
0.0
30.0
60.0
90.0
120.0
150.0
180.0
210.0
time
4.80
5.20
5.60
6.00
6.40

CONCLUSIONS

1) TIME RESOLUTION IN THE μs RANGE WILL BE FEASIBLE IN SINGLE-SHOT EXPERIMENTS, FOR CRYSTALS LIKE MYOGLOBIN, WITH APS/ESRF/CHESS UND.

I.E. THE X-RAYS, FROM ONLY A FEW - OR EVEN ONE - BUNCH YIELD SUFFICIENT SIGNAL IN A LAUE EXPERIMENT.

IF ONE BUNCH, THE TRUE TIME RESOLUTION IS THE X-RAY PULSE LENGTH ~ 100 ps

2) TIME-RESOLVED DETECTION IS A PROBLEM!

- INTEGRATING DETECTORS?

3) REACTION INITIATION IS A PROBLEM

E.G. $t_{1/2}$ FOR PHOTOLYSIS OF CAGED ATP IS ~ 4 ms

BUT IR LASER? T-JUMP? PRESSURE JUMP?

I.E. PHYSICAL INITIATION, NOT CHEMICAL

WORKSHOP REPORTS

X-RAY AND NEUTRON SCATTERING FROM MAGNETIC MATERIALS*

Doon Gibbs
Brookhaven National Laboratory

On November 6-7, 1987, a workshop was held at Argonne to discuss technical and scientific advances in the study of magnetic materials by x-ray and neutron scattering techniques: the complementarity of the two kinds of probes, their relative strengths, and recent developments. This was the first workshop, I believe, to combine x-ray and neutron scattering studies of magnetic materials, at least in the context of magnetic x-ray scattering, and it attracted 100 people from all over the world. The meeting organizers were Jerry Lander, Harold Myron, and myself. The workshop was opened by David Moncton, and the first speaker was Ken Kliewer, who discussed the complementarity of x-ray and neutron scattering.

The first session had as its common denominator surface magnetism and multilayers. The afternoon session was largely devoted to x-ray and neutron polarization dependence, with a couple of high-Q resolution talks as well. There were talks on nuclear Bragg scattering, and the last session dealt with high-T_c superconducting materials.

I would like now to present a few details about magnetic x-ray scattering per se and indicate some possible uses at the Advanced Photon Source.

In principle, one can separate the orbital and spin densities in an x-ray scattering experiment. This is not the case in neutron scattering. There is an interference term that is nonzero only when the Bragg peaks and the magnetic peaks come at the same position in reciprocal space, but then something has to be done to extract the magnetic scattering -- typically, a magnetic field is introduced. If you align the spin in the direction of the field, measure the Bragg intensity and then change the field, the spin dependence can be isolated. Thus, one can directly study ferromagnetic structures, as well as antiferromagnetic ones, with x-rays.

I would like to discuss some new results involving polarization dependence and resonance in holmium. If you separately measure the parallel and perpendicular components of a linearly polarized beam incident on a sample, it is possible to separate the orbital and spin magnetization densities directly. In fact, this applies generally to arbitrary magnetic structures, and it can be done for any incident polarization. The technique is still not sensitive enough to extract the Q dependence of the ratio of orbital and spin densities in holmium; that situation can be improved by increasing the linear polarization of the incident beam, something of importance at APS. Most ferromagnetic materials are studied using circular polarization, so what one would really like to have is a beam line with tunable polarization.

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*The summary presented here is based on notes taken at the meeting.

A second example involves the energy dependence of the magnetic x-ray scattering cross-section in holmium. There is a 50-fold increase in the scattering intensity at the L3 edge. You also get harmonics at values where the usual picture of holmium's magnetic structure would forbid them; these are resonance effects. The resonant line shape is really a probe of excited magnetic states in holmium vs. energy. Results such as these open up a new range of possible studies.

Synchrotron-based experiments on magnetic x-ray scattering performed in the last 15 years have covered a range of materials -- transition metals, rare earths, iron chromium, superlattices -- and difference techniques -- spin-dependent Thompson scattering, interference techniques, and pure studies of magnetic scattering in antiferromagnetic magnets. High-Q resolution will be at an advantage at the APS. Such facilities will also be particularly useful for investigating sensitivity to lattice modulations in rare earth metals, a unique polarization dependence that allows separation of orbital and spin densities, and novel resonance and interference effects. The beam is naturally small, an advantage in studying small samples. The scattering is so weak there is essentially no extinction in the magnetic scattering. In fact, with properly designed beam lines the incident polarization and energy could be tunable, permitting a whole range of new experiments: detailed magnetic structure determinations, separation of spin and orbit in ferromagnets and antiferromagnets, resonant spectroscopy, and possibly even surface magnetic x-ray scattering.

X-RAY SYNCHROTRONS AND DEVELOPMENT OF NEW MATERIALS*

Stephen Durbin
Purdue University

The Advanced Photon Source Users Organization sponsored a workshop, "X-Ray Synchrotrons and the Development of New Materials," at Argonne National Laboratory on December 10-11, 1987. This workshop focused on two issues: (1) how materials research at existing x-ray synchrotrons has advanced the understanding and development of new materials and (2) how the Advanced Photon Source (APS) can be optimized to stimulate the science and technology of new materials. Presentations described the broad range of materials requiring an x-ray synchrotron source for the investigation of important properties. Much of the research using synchrotron radiation has been directed toward improving the understanding of existing materials and the engineering of new materials with specific physical properties having technological applications. Discussions of new materials that have resulted from synchrotron-radiation-based research (e.g., Fibonacci superlattices, ultra-high pressure phases, catalysts, etc.) indicated that the APS can become an important part of the process of developing new materials.

Specific recommendations by workshop participants for materials research on APS beam lines included the following:

- A high-brightness undulator beam line should be dedicated to extremely high-resolution diffraction measurements of single crystals.
- A second high-brightness undulator should be dedicated to high-resolution powder diffraction measurements to permit structural determinations of materials that cannot be prepared as single crystals.
- A dedicated wiggler source should provide high fluxes over a large energy range for extended x-ray absorption fine-structure (EXAFS), surface extended x-ray absorption fine-structure (SEXAFS), and x-ray absorption near edge structure (XANES) spectroscopy. This wiggler source would provide maximum sensitivity for absorption determinations of electronic and structural properties for a wide range of materials.

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*Summary based on workshop organizers' Executive Summary in "X-Ray Synchrotrons and the Development of New Materials: Workshop Report," Argonne National Laboratory Report ANL/APS-TM-1 (Feb. 1988).

X-RAY SYNCHROTRONS AND NEW OPPORTUNITIES IN THE EARTH SCIENCES*

Joseph Smith
The University of Chicago

On January 18-20, 1988, a workshop entitled "X-Ray Synchrotrons and New Opportunities in the Earth Sciences," sponsored by the APS Users Organization, Argonne National Laboratory's Division of Educational Programs, and The University of Chicago, was held at Argonne. The workshop was devoted to presentations in four principal areas of research involving the use of synchrotron radiation: (1) x-ray scattering studies, including diffraction, on very small single crystals, powders, noncrystalline materials (glasses, melts, liquids, metamict materials) and mineral surfaces and interfaces, as well as studies of transient phenomena requiring time-resolved measurements; (2) x-ray scattering studies on minerals and melts at ultra high pressures (up to 500 GPa) and temperatures (up to 7000 K); (3) x-ray spectroscopy studies, including x-ray absorption, emission, and photoelectron spectroscopy, on minerals, melts, glasses, liquids, and interfaces; and (4) x-ray fluorescence microprobe analyses of a wide range of natural materials. The first three areas primarily involve structure-property relationships, while the fourth area is concerned with compositional variations in solid earth materials.

At the workshop, an organization -- named "GeoSync" -- was established to promote and coordinate research in the geosciences using synchrotron radiation. The establishment of Geosync marks the beginning of what it is hoped will be a very active and productive program for the use of the APS in research on earth materials.

*Summary based on Executive Summary and Introduction in "Synchrotron X-Ray Sources and New Opportunities in the Earth Sciences: Workshop Report," Argonne National Laboratory Report ANL/APS-TM-3 (April 1988).

TIME-RESOLVED STUDIES AND ULTRAFAST DETECTORS*

Paul Sigler
The University of Chicago

Participants in a workshop on "Time-Resolved Studies and Ultrafast Detectors," held at Argonne National Laboratory on January 25-26, 1988, discussed new avenues in time-resolved research that will be opened by the Advanced Photon Source (APS). The APS will provide an enormous enhancement in brilliance over existing x-ray sources, dramatically increasing capabilities for the extension of static x-ray techniques into the time domain, with timescales from milliseconds to picoseconds. Interest in time-resolved measurements spans the materials and biological sciences, from semiconductors to metalloproteins, and the whole area represents a major frontier for synchrotron radiation research. Working groups considered the physical characteristics of the source that would be crucial for successful experiments. Also discussed were the experimental difficulties to be overcome, such as uniform excitation of samples and development of improved detectors. Presentations by detector designers and builders outlined current technologies and indicated future research directions.

One of the most exciting opportunities offered by the new generation of synchrotron x-ray sources is the ability to do single-pulse experiments. Such experiments are feasible with insertion devices capable of supplying more than 10^9 photons in a single subnanosecond burst at greater than 1% bandwidth. Speakers identified electron transfer mechanisms in photosynthetic reactions and metal-ligand bonding in proteins as examples of areas in which the time structure of the synchrotron source could be important.

Detector shortcomings appear to be a limiting factor in much of the work now under way at existing synchrotron facilities. Without concerted effort, detection schemes will be inadequate for taking advantage of the high fluxes and novel temporal characteristics of new sources like the APS. Virtually every workshop speaker remarked on this problem.

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*Summary based on Abstract and Introduction in "Time-Resolved Studies and Ultrafast Detectors: Workshop Report," Argonne National Laboratory Report ANL/APS-TM-2 (Feb. 1988).

REPORTS ON R&D AT OTHER
SYNCHROTRON FACILITIES

R&D AT SSRL IN SUPPORT OF THE ADVANCED PHOTON SOURCE*

Herman Winick
Stanford Synchrotron Radiation Laboratory

Many activities at SSRL are relevant to the APS and can therefore be considered R&D in support of the APS. This includes work on SPEAR on beam steering and stability, insertion-device development, and the development of beam-line optics and monochromators that can function under high thermal loading.

The work on PEP is even more relevant, because the PEP ring and the two operational undulator beam lines on PEP can now perform at levels approaching the performance levels planned for the APS. This talk therefore concentrates on the work done on PEP, particularly the low-emittance 7.1-GeV run that took place over December 9-21, 1987. Accelerator physicists from the APS, as well as from other facilities, participated in this run. The excellent results achieved on the run are due to the fine cooperation and contributions of more than 20 scientists from five laboratories. We look forward to continued collaborations in the future.

Recently, a new concept for a reliable, simple, inexpensive vacuum chamber for use with insertion devices was suggested by Richard Boyce of SSRL. The concept is being developed in collaboration with James Viccaro of the APS. E. Hoyer of LBL and Henry Halama of NSLS are also involved. The basic concept is shown in the figures. If such a chamber were successfully developed, it would have a major impact on the effective utilization of the APS, because it would make large apertures available for injection and smaller apertures for the stored beam, thus facilitating the use of the smallest undulator gaps consistent with good lifetime.

A joint project between APS, SSRL, and also LBL and NSLS is proposed to design and build a prototype of such a chamber that could be tested in PEP along with the APS/CHESS 3.3-cm-period undulator.

*The following statement and copies of viewgraphs were provided by the speaker.

PEP

as a Synchrotron Radiation Source

Basic Characteristics

- High Energy: 16 GeV
- Long Straight Sections: 6 x 117 m
  6 x 5.5 m
- Large Circumference: 2200 m
- Low Bend Magnet Field: 0.32 T @ 16 GeV

FLEXIBILITY !!

- Low emittance
- High Photon Energy
- Long Undulators
- Short Pulses
- High Peak Power
- Special Polarization

H. Winick
SSRL
March 10, 1988

PEP offers "next generation" capabilities now and has the potential to go to even higher performance levels.

- Gain early experience with "next generation" sources (APS, ALS, ESRF, Japan, ...)
- Test-bed for a future 21st century diffraction-limited X-Ray ring

Workshop on PEP as a Synch. Rad. Source
Oct 20-21, 1987
Report available from SSRL

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APS/PEP Cooperation/Collaboration

- Operations experience with a low emittance 7 GeV ring
- Testing monochromators, beam line optics, other components
- Insertion device development and operations experience; e.g., use of APS/CHESS undulator on PEP
- Variable gap vacuum chamber development and testing

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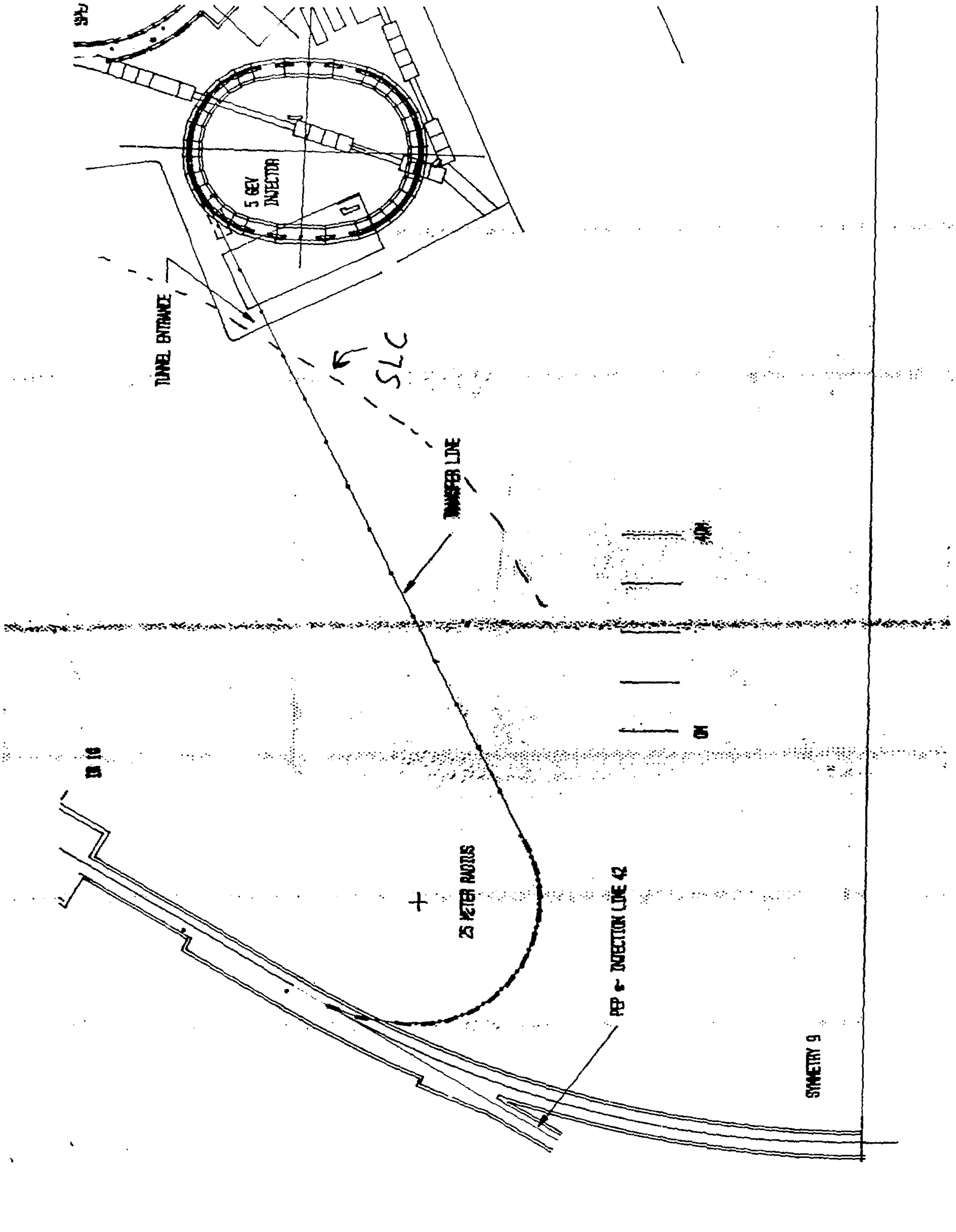


TUNNEL ENTRANCE
5 GEV INJECTOR
SLC
TRANSFER LINE
25 METER RADIUS
PEP e- INJECTION LINE 42
SYMMETRY 9

PEP

Long Straight Sections

(117 m)

Uses:

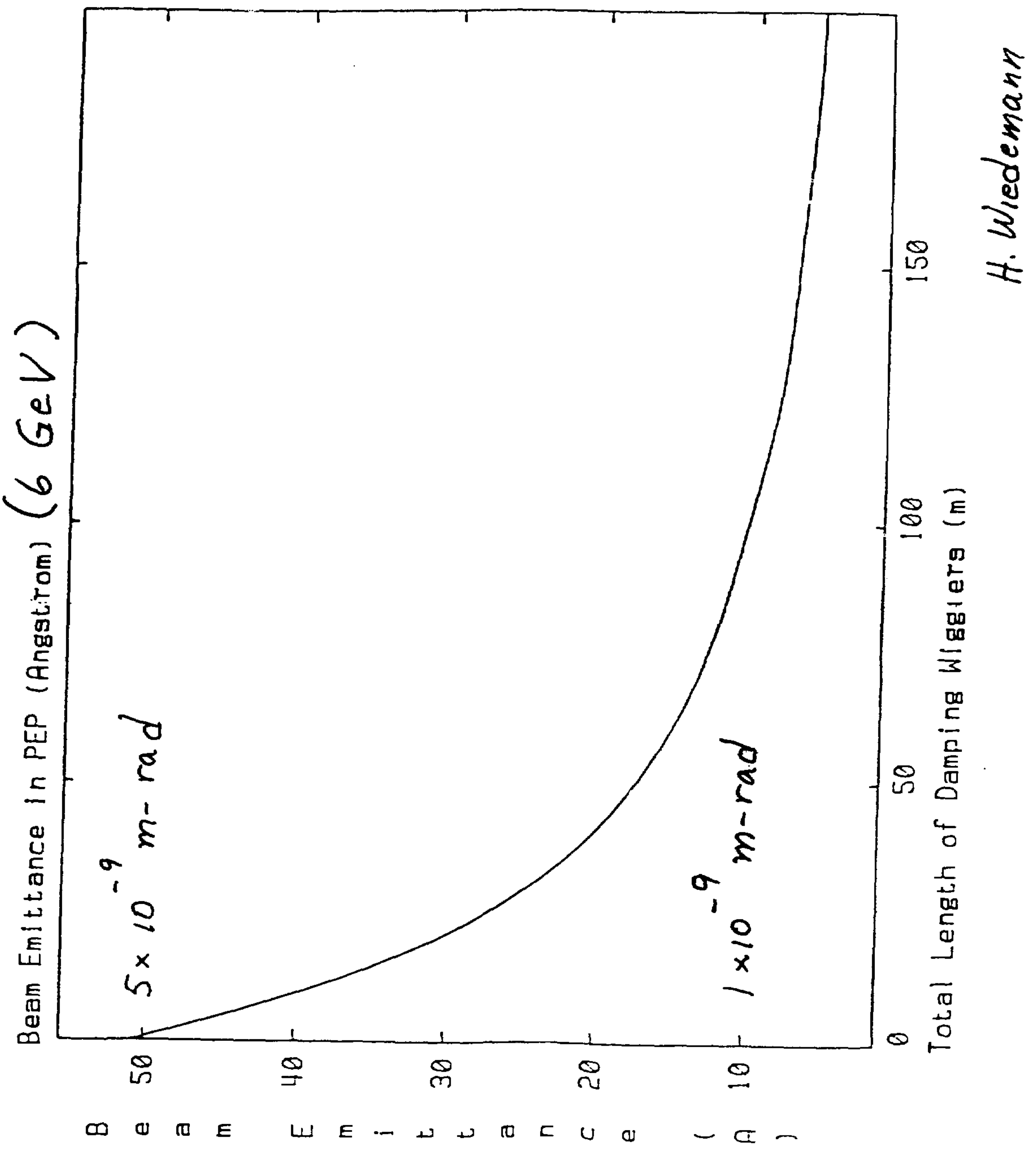
1. Damping Wigglers: Achieve ultra-low emittance (<10^{-9} m-rad), highest brilliance, high coherent power (Wiedemann)

2. Long Insertion Devices: e.g. proposed 12 m undulator

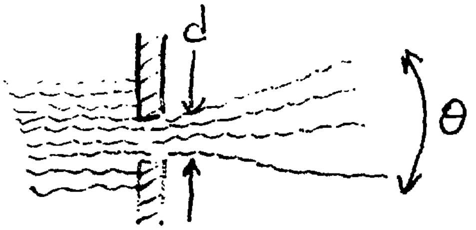
3. Chicane Beam Lines: 2-4 beam lines in each long straight

4. Bypass: To accommodate special insertion devices.

Long straight sections of PEP have zero dispersion - no broadening of source size due to energy spread


Beam Emittance In PEP (Angstrom) (6 GeV)
5×10-9 m-rad
1×10-9 m-rad
Beam Emittance (A)
50
40
30
20
10
0
50
100
150
Total Length of Damping Wigglers (m)
H. Wiedemann

How Low can the Photon Beam Emittance Be?



Diffraction sets the limit

$$d \cdot \theta \gtrsim \lambda$$

For a Gaussian distribution

$$\epsilon_{x\gamma} = \sigma_{x\gamma} \cdot \sigma_{x'\gamma} \geq \lambda / 4\pi = \text{Minimum Photon Beam Emittance}$$

There is no gain in brilliance of the light if the electron beam emittance is reduced below $\lambda / 4\pi$.

Examples

$h\nu$ (eV)	10	100	1,000	10,000
λ (nm)	124	12.4	1.24	0.124
ϵ (nm-rad) (diffraction Limit)	10	1	0.1	0.01

PARTICIPANTS IN THE DECEMBER, 1987 PEP LOW EMITTANCE RUN

ADVANCED LIGHT SOURCE (LBL): Alan Jackson, Michael Zisman

ADVANCED PHOTON SOURCE (ANL): Stephen Kramer, Moohyun Yoon

NATIONAL SYNCHROTRON LIGHT SOURCE (BNL): Ben Craft, Glenn Decker, John Galayda

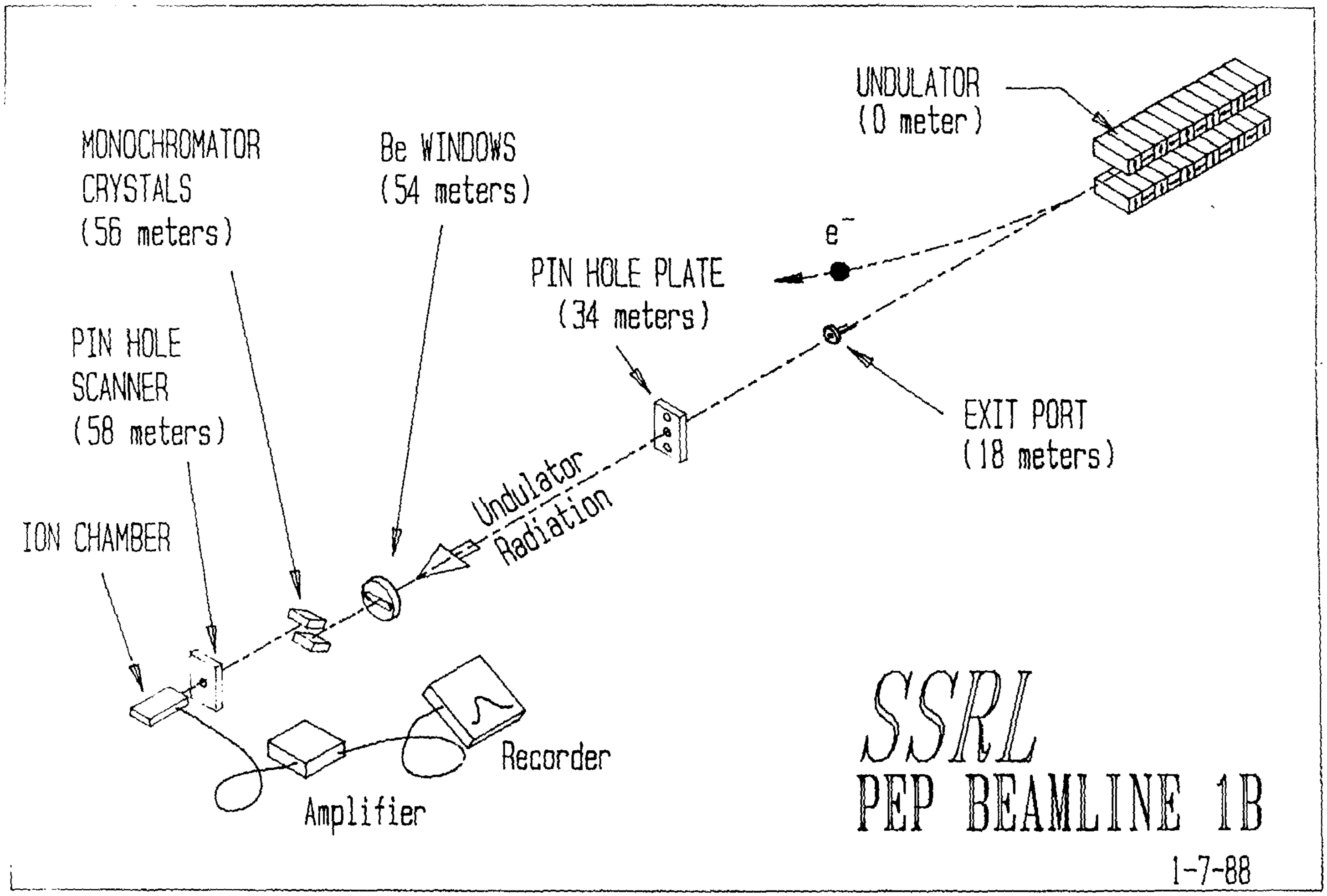
SLAC: Matthew Allen, Elliott Bloom, Martin Donald, Ewan Paterson, Jean-Louis Pellegrin, Burton Richter, Leonid Rivkin, Heinz Schwarz

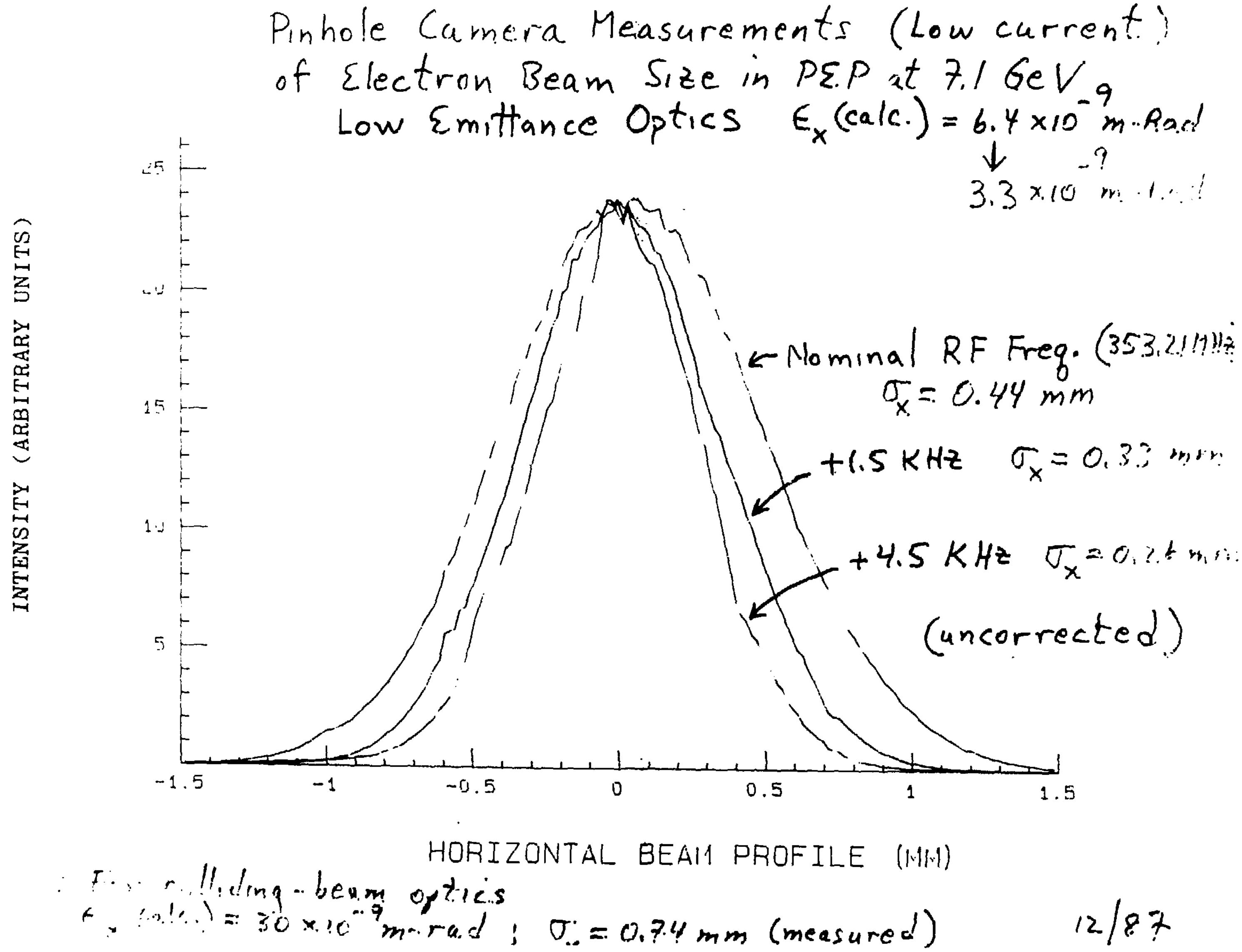
SSRL: George Brown, Roberto Coisson, Robert Hettel, Teresa Troxel, Helmut Wiedemann, Herman Winick

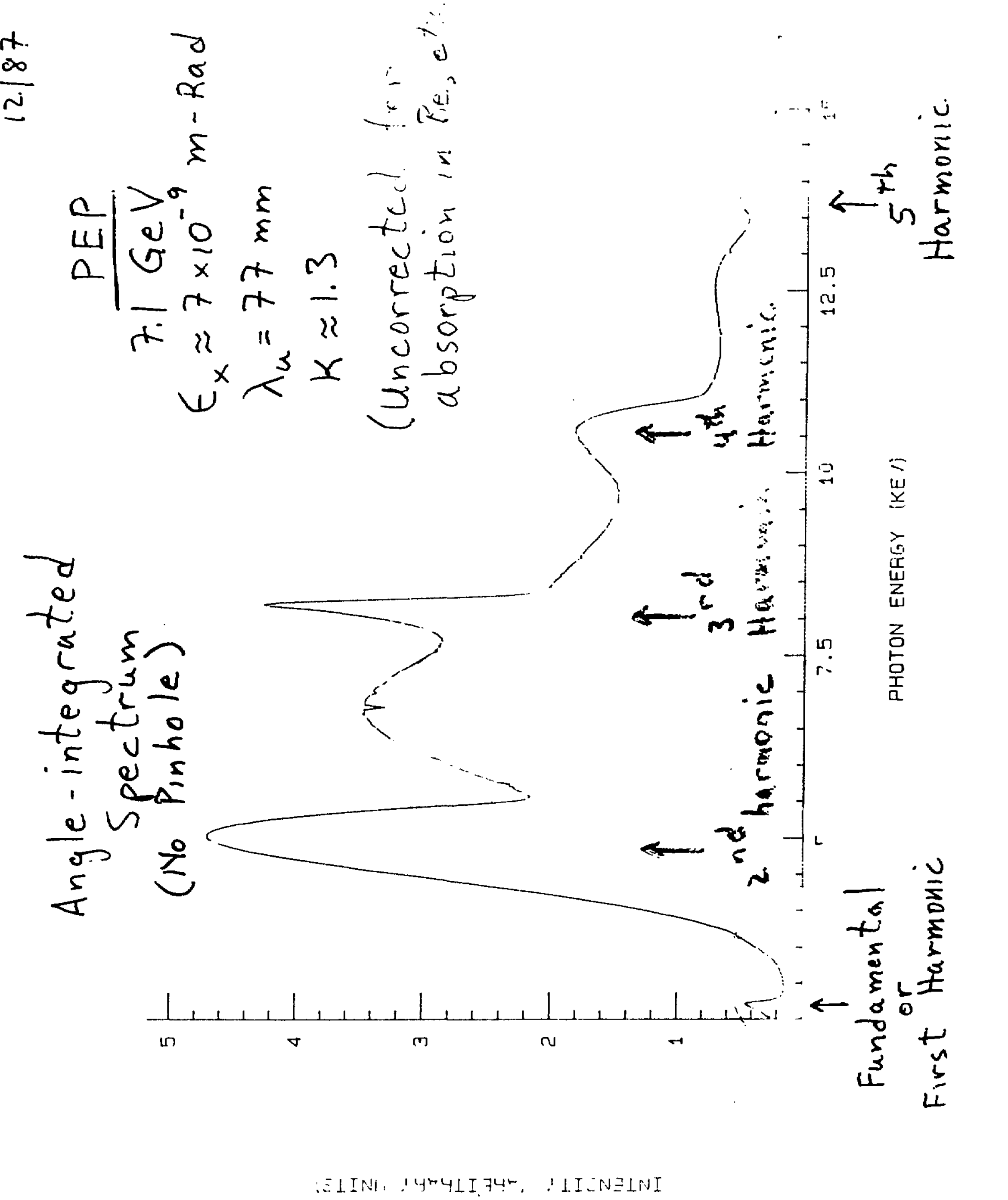
STANFORD/SSRL GRADUATE STUDENTS: Michael Borland, Louis Emery, William Lavender, James Safranek, Wanfen Xie

Low Emittance PEP Run 12/9-21/87

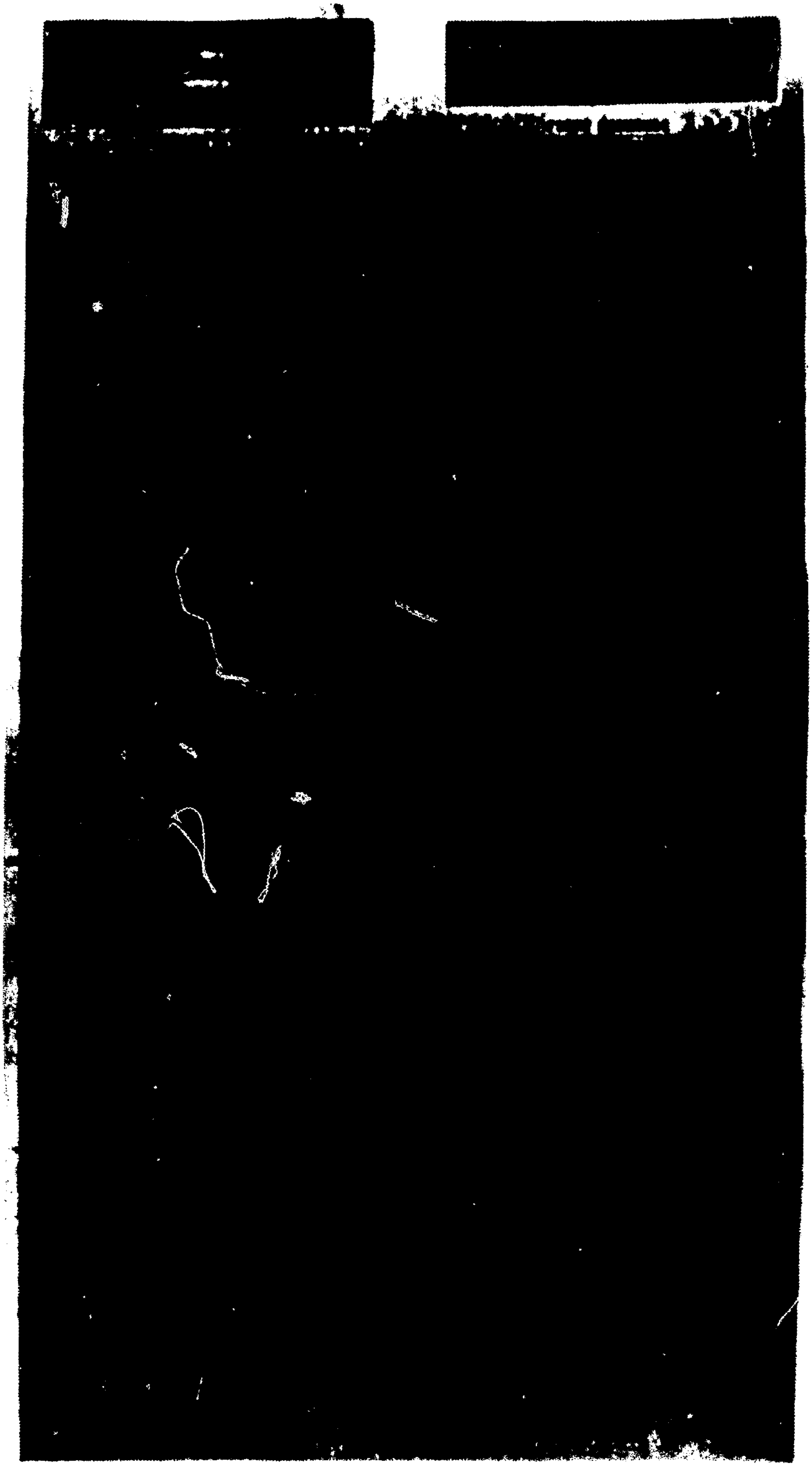
- Low emittance optics implemented & characterized
- Calculated emittance at 7.1 GeV
  - 6.4×10^{-9} m-rad; normal damping partition
  - 3.3×10^{-9} m-rad; changed damping partition
- Stored current
  - 33 mA; maximum achieved
  - 10-15 mA; better stability & reproducability
- Lifetime; 2-3 hours
- Studied single & multi-bunch instability limits. Implemented counter-measures to raise thresholds
- Commissioned 2nd Undulator beam line
  - Many spectra under different conditions
  - Pinhole x-ray camera implemented
  - Photon beam steering/stabilization system characterized
- Studied injection aperture requirements

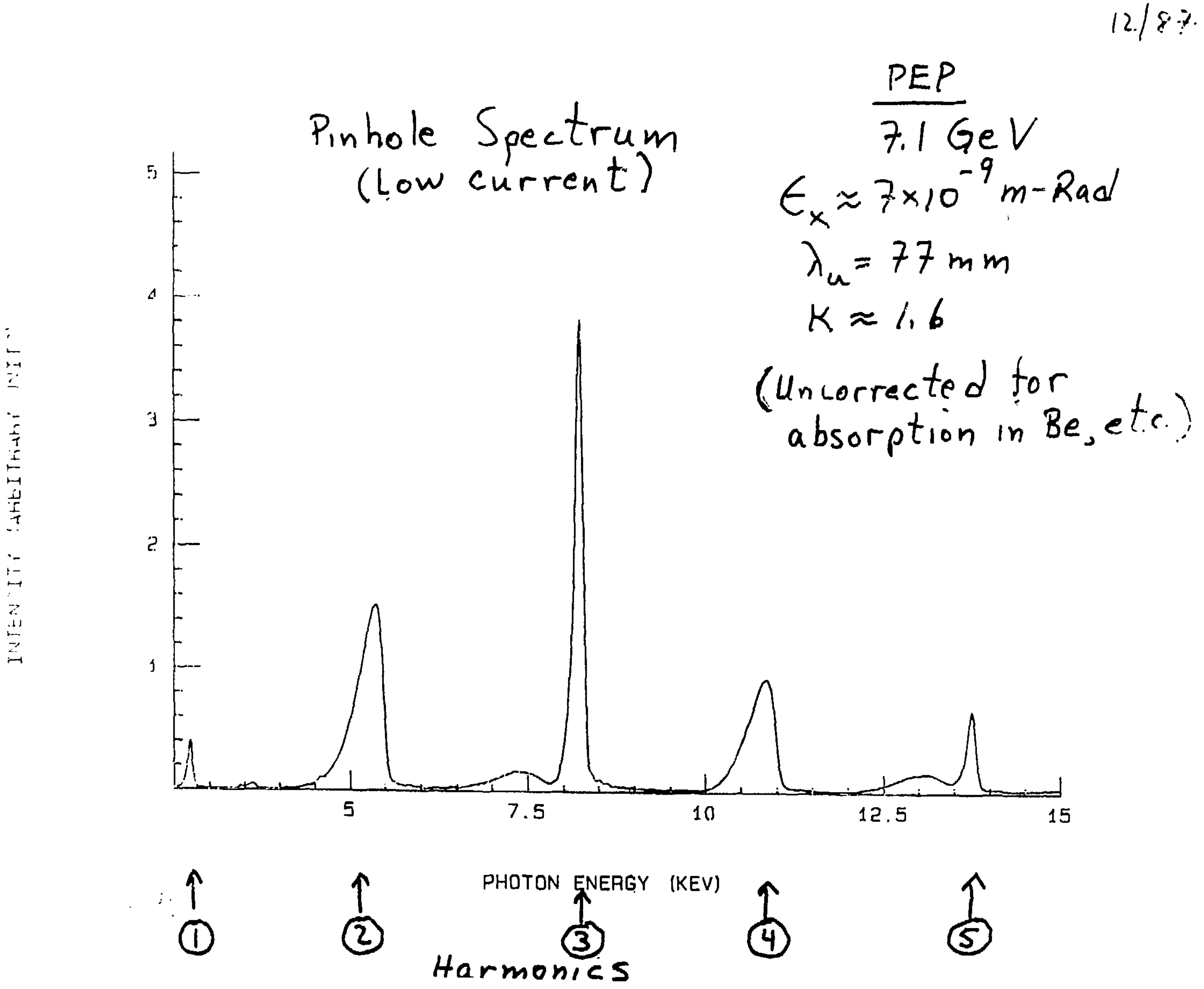

UNDULATOR
(0 meter)
MONOCHROMATOR
CRYSTALS
(56 meters)
Be WINDOWS
(54 meters)
e⁻
PIN HOLE PLATE
(34 meters)
PIN HOLE
SCANNER
(58 meters)
EXIT PORT
(18 meters)
Undulator
Radiation
ION CHAMBER
Recorder
Amplifier
SSRL
PEP BEAMLINE 1B
1-7-88


Pinhole Camera Measurements (Low current)
of Electron Beam Size in PEP at 7.1 GeV
Low Emittance Optics E_x(calc.) = 6.4 x 10^{-9} m-Rad
3.3 x 10^{-9}
INTENSITY (ARBITRARY UNITS)
5
15
25
-1.5
-1
-0.5
0
0.5
1
1.5
HORIZONTAL BEAM PROFILE (MM)
← Nominal RF Freq. (353.21MHz)
σ_x = 0.44 mm
+1.5 KHz
+4.5 KHz
(uncorrected)
-beam optics
= 30 x 10^{-9} m-rad ; = 0.74 mm (measured)
12/87

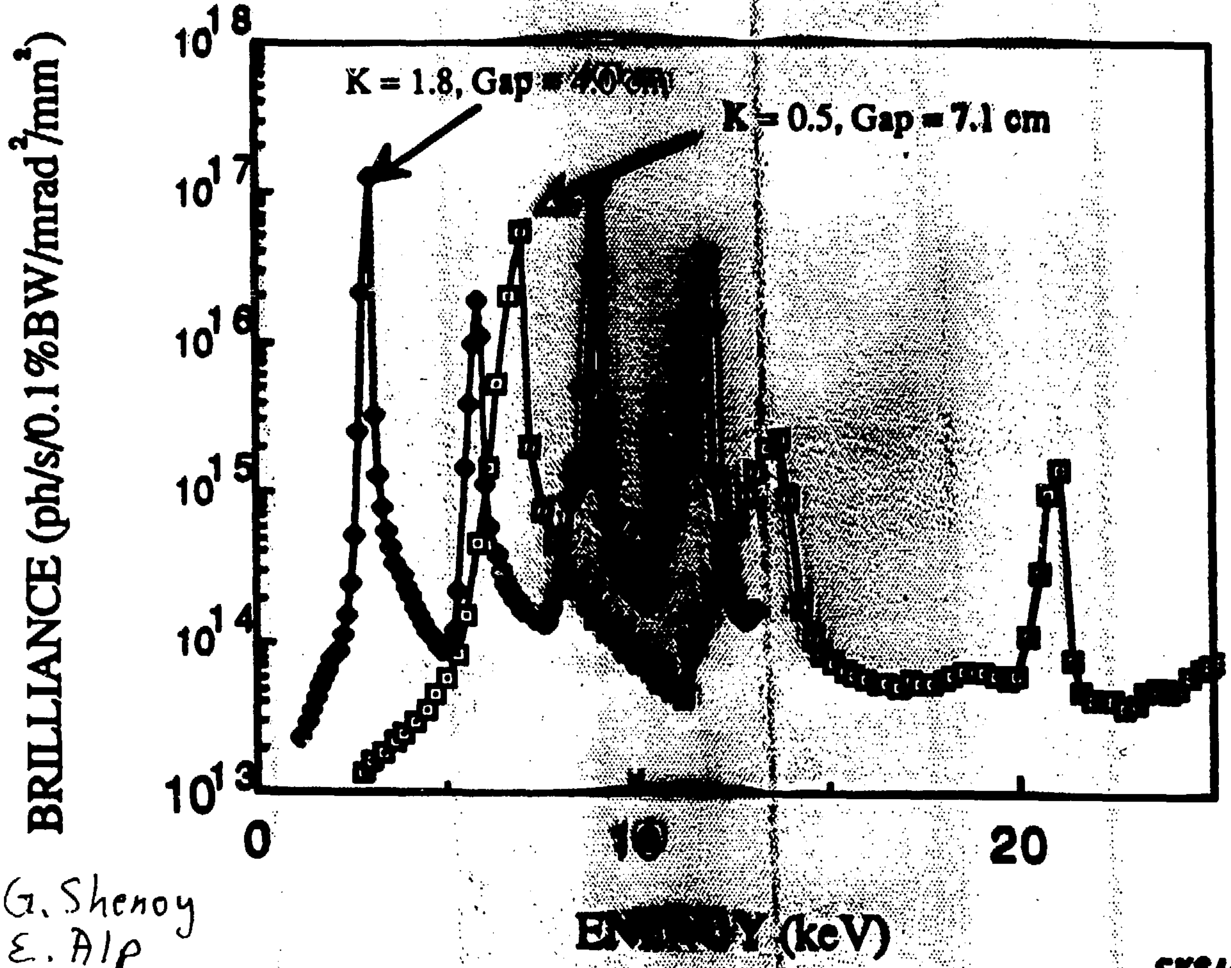


12/87
Angle-integrated Spectrum (No Pinhole)
PEP
7.1 GeV
$E_x \approx 7\times10^{-9}$ m-Rad
$\lambda_u = 77$ mm
$K \approx 1.3$
(Uncorrected
absorption in
Fundamental or First Harmonic
2nd harmonic
3rd Harmonic
4th Harmonic
5th Harmonic
PHOTON ENERGY (KEV)
7.5
10
12.5
1
2
3
4
5




12/87
Pinhole Spectrum
(Low current)
PEP
7.1 GeV
$\epsilon_x \approx 7\times10^{-9}$ m-Rad
$\lambda_u = 77$ mm
$K \approx 1.6$
(Uncorrected for
absorption in Be, etc.)
5
4
3
2
1
5
7.5
10
12.5
15
PHOTON ENERGY (KEV)
1
2
3
4
5
Harmonics

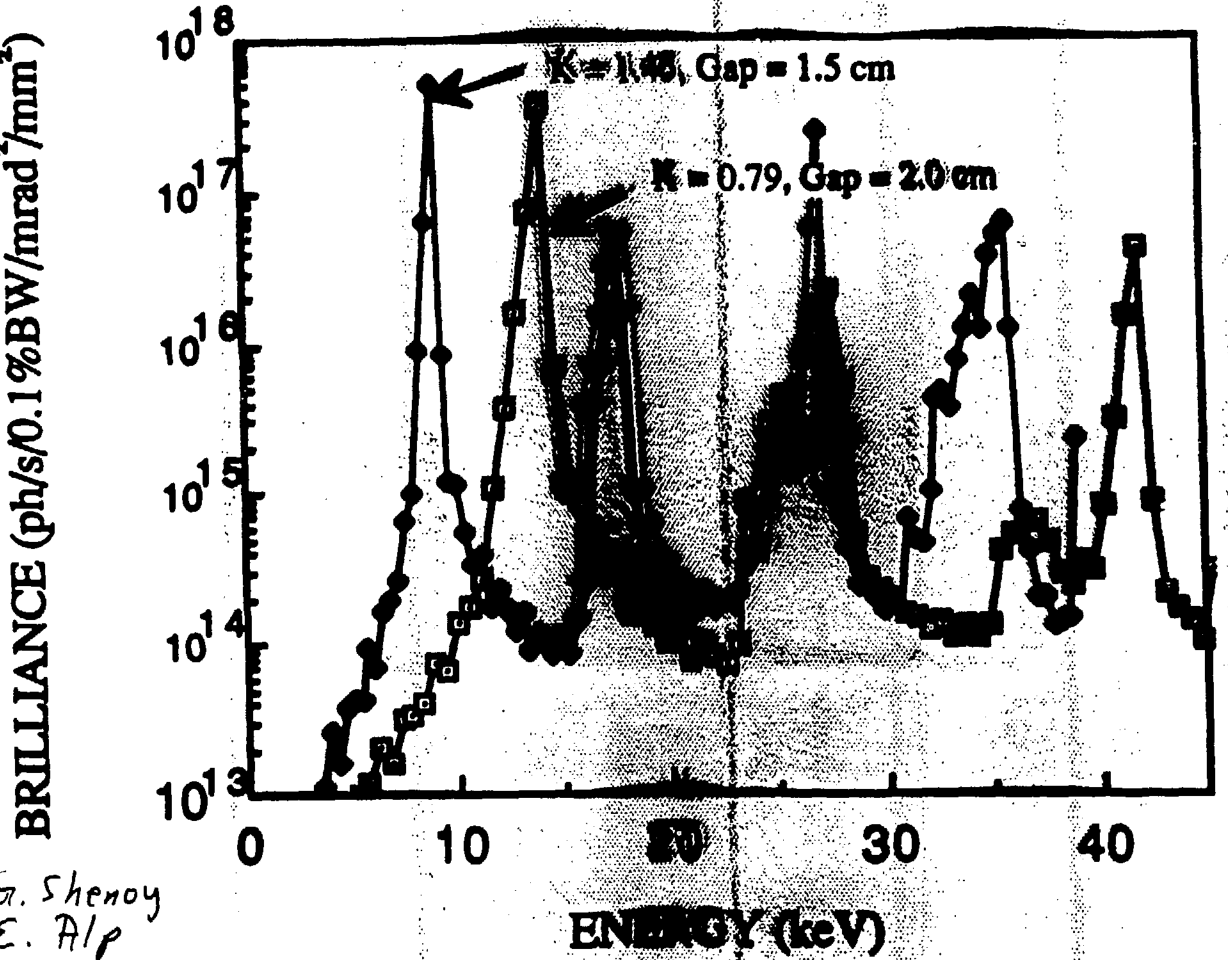
PEP/8 GeV/100 mA/LEO/REC 7.7 cm/N = 26



G. Shenoy
E. Alp
T. Viccaro

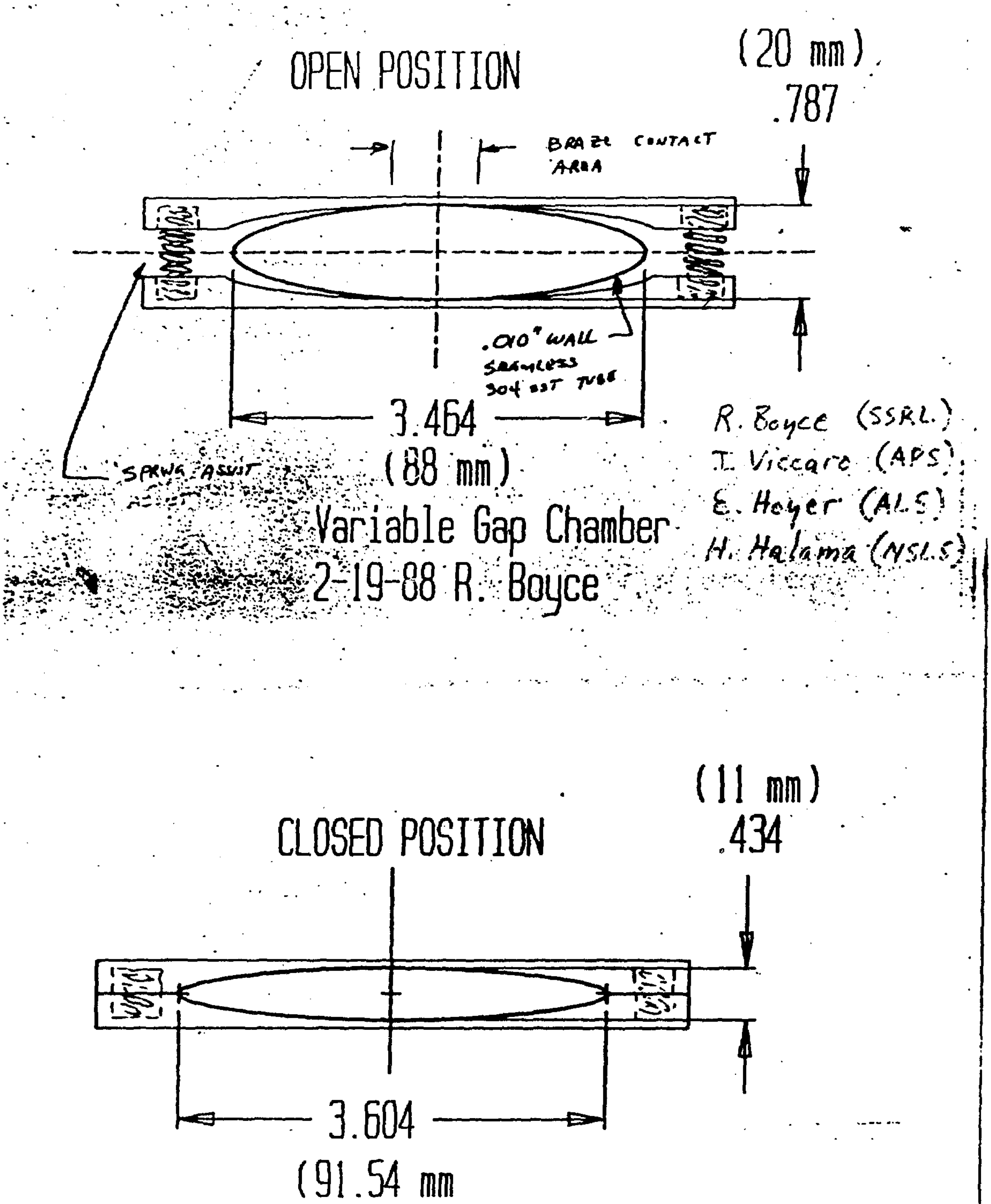
GKS/ANL/OCT87

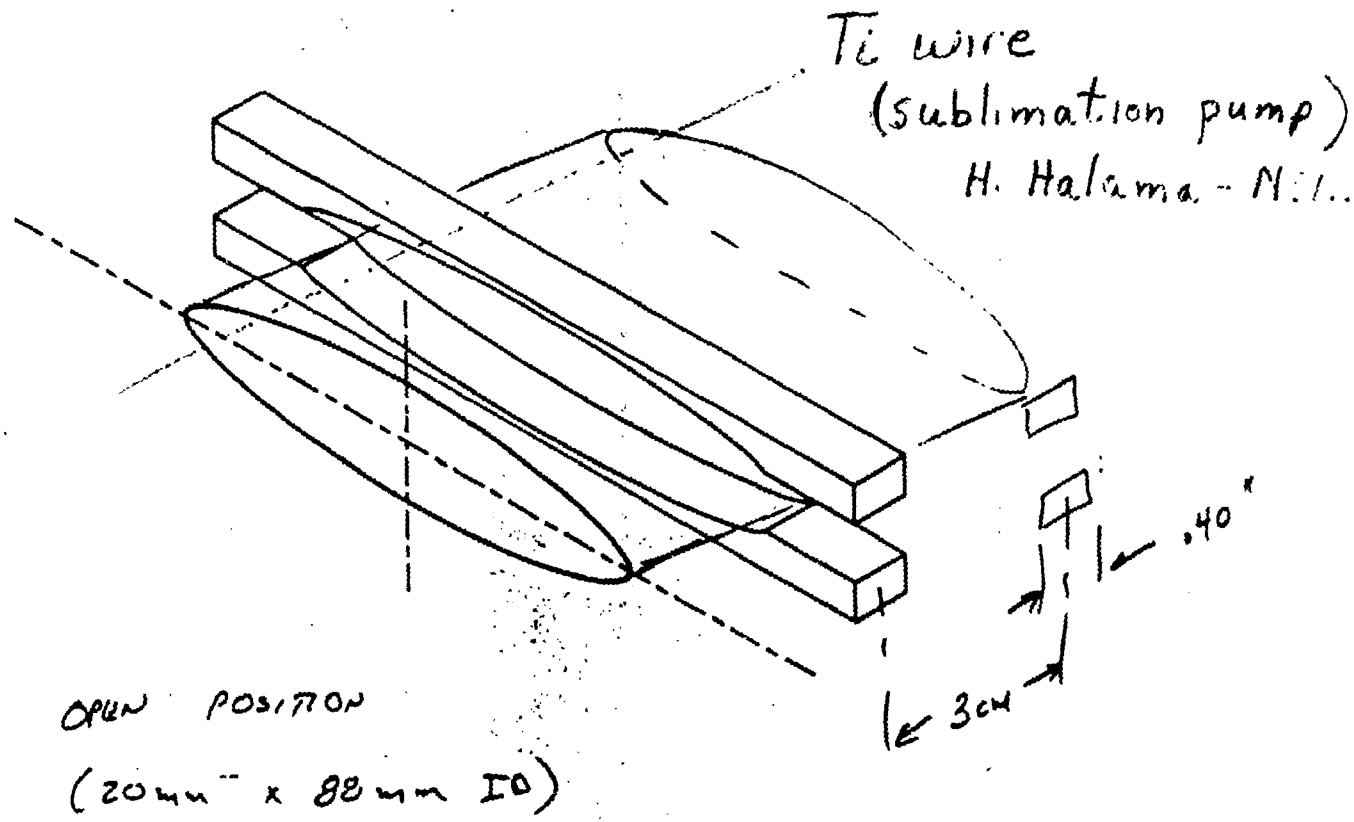
PEP/8 GeV/100 mA/LEO/Nd-Fe-B 3.3 cm/N = 60



G. Shenoy
E. Alp
J. Viccaro

GKS/ANL/OCT87


OPEN POSITION
(20 mm)
.787
BRAZE CONTACT AREA
.010" WALL SEAMLESS 304 SST TUBE
3.464
(88 mm)
R. Boyce (SSRL)
J. Viccaro (APS)
E. Hoyer (ALS)
H. Halama (NSLS)
Variable Gap Chamber
2-19-88 R. Boyce
CLOSED POSITION
(11 mm)
.434
3.604
(91.54 mm



Ti wire
(sublimation pump)
H. Halama
.40"
3cm
OPEN POSITION
(20mm x 88mm ID)

2-19-88

Future Operation of PEP

Determined by Budget

Up to 7-8 months/yr parasitic

2-3 months/yr dedicated

(statement by B. Richter at PEP Wkshop)

Near term plan

August - November, 1988; Colliding Beams

December, 1988 - Jan, 1989; Synch. Rad.

Future Directions for Synch. Rad.

I - New 6-10 GeV dedicated rings
(APS, ESRF, JAPAN)

- Ready in mid-1990's
- Emittance $\sim 5 \times 10^{-9}$ m-rad
- Provide 10^{18}-10^{19} level of brightness to large User community on many beam lines
- Provide reliable, stable operation for many hours/year.

II - Large e^+/e^- colliders used as sources of Synch. Rad. (PEP [16 GeV], Tristan [30 GeV])

- Could provide $\sim 5 \times 10^{-9}$ m-rad now
- Gain early experience with 10^{18}-10^{19} level of brightness
- Flexibility for future development
  - High electron energy
  - Large circumference
  - Long straight sections

CHESS SUPPORT FOR APS*

Michael Bedzyk
Cornell University

From CHESS:

D. Bilderback
C. Henderson
M. Bedzyk
Q. Shen
D. Mills‡
K. Finkelstein
W. Schildkamp
B. Batterman

From ANL:

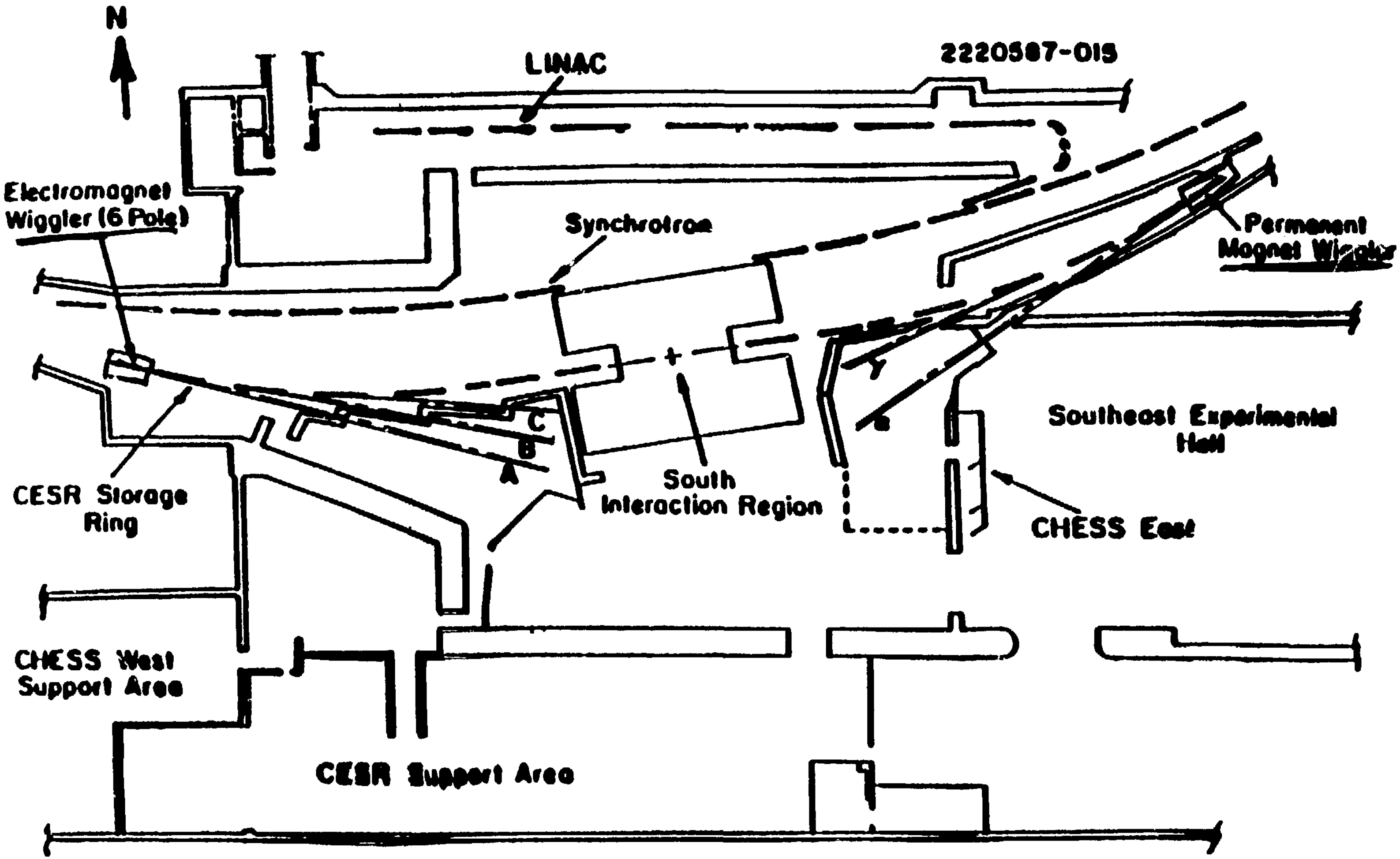
G. Shenoy
R. Smither
J. Viccaro
D. Moncton
D. Mills‡

From CESR:

E. Blum
D. Hartell

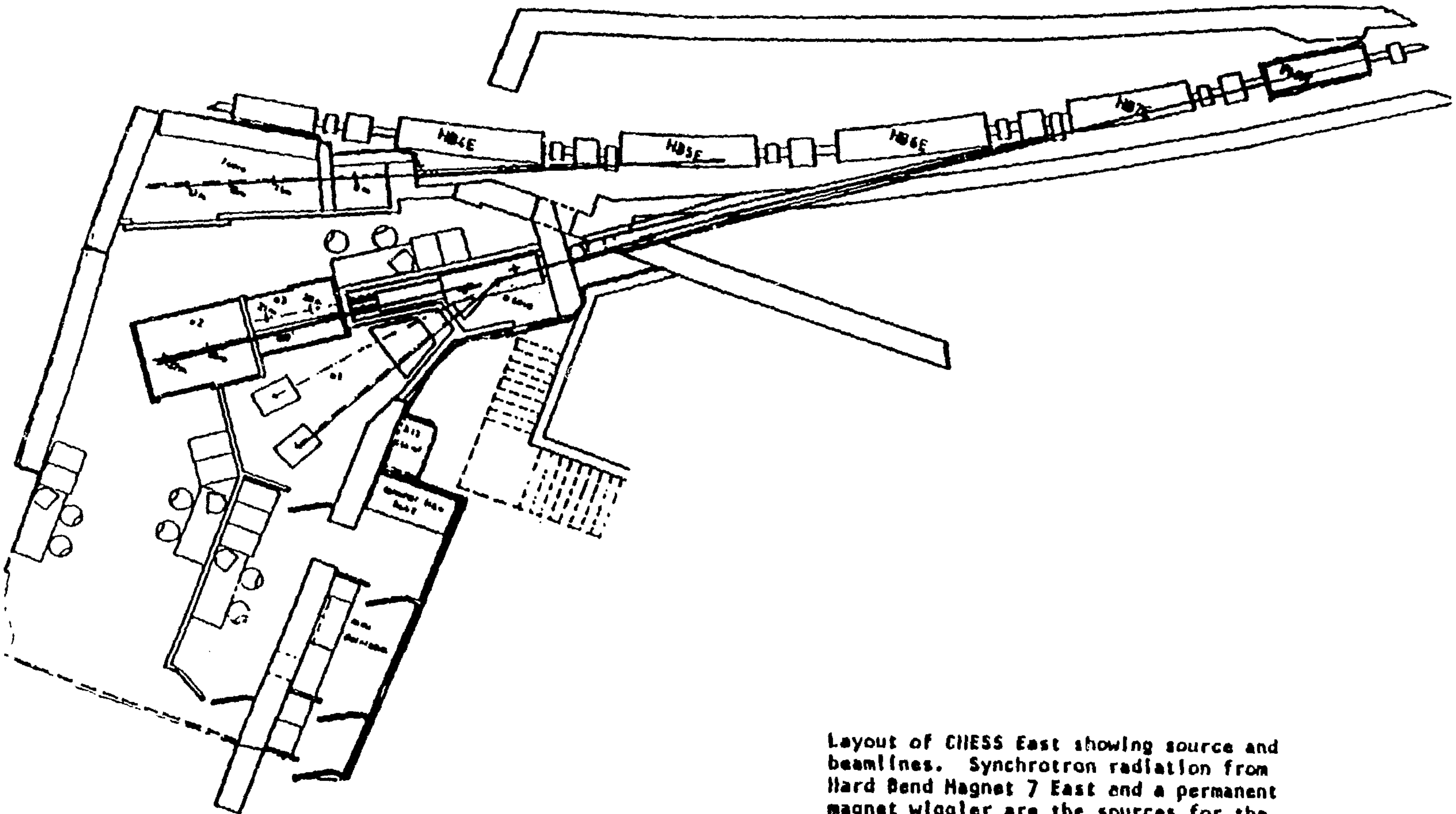
*The following copies of viewgraphs were provided by the speaker.

‡On leave from CHESS, Cornell University.

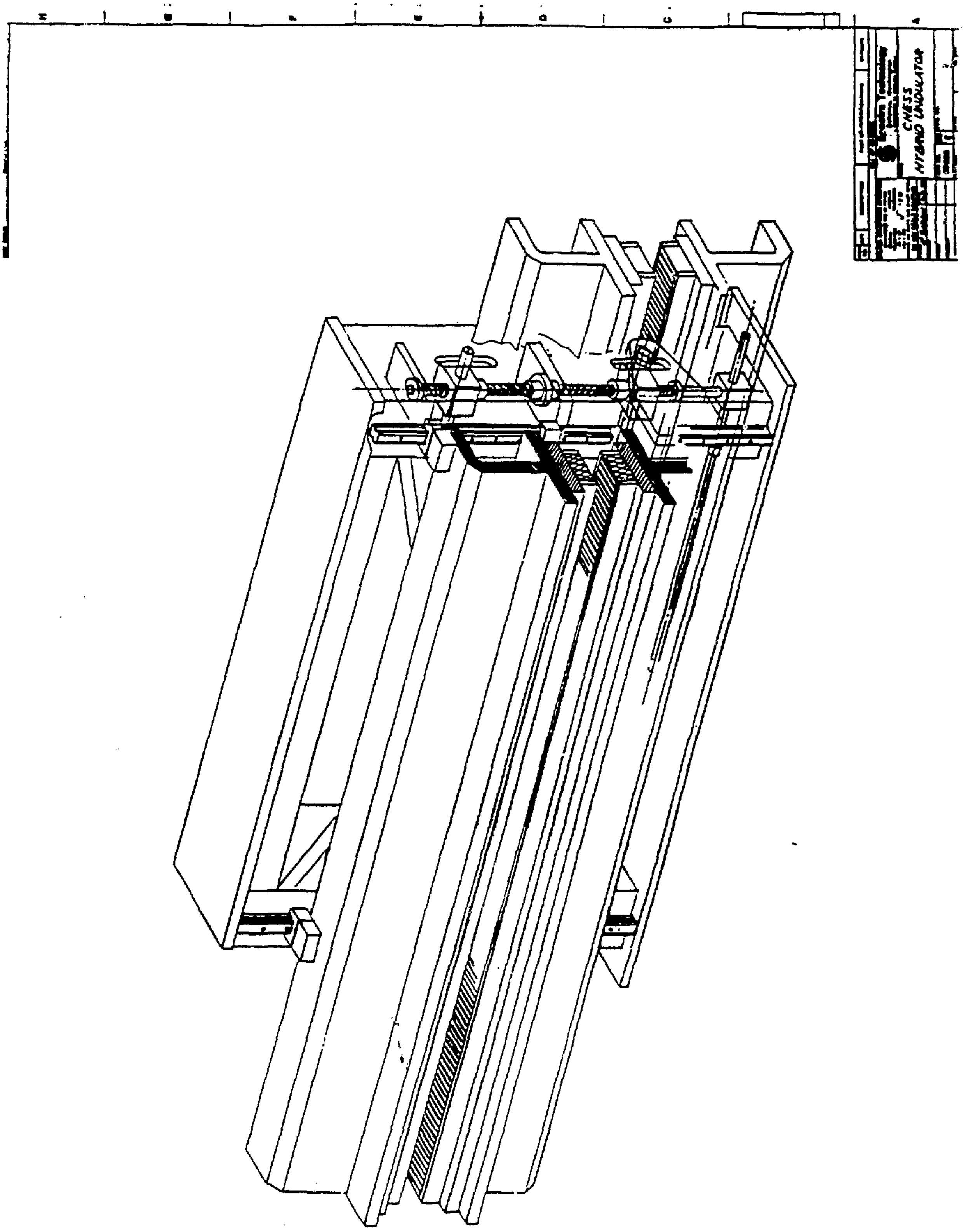


Schematic of the synchrotron radiation facility shown in relation to the high energy experimental halls. The present synchrotron radiation beamlines and support area are denoted as CHESS West. The new CHESS East development will occupy floor space just to the East of the South Interaction Region.

CHESS EAST



Layout of CHESS East showing source and beamlines. Synchrotron radiation from Hard Bend Magnet 7 East and a permanent magnet wiggler are the sources for the Alpha line. The Gamma line receives its radiation from Hard Bend Magnet 5 East.


CHESS
HYBRID UNDULATOR

CHESS / ANL UNDULATOR

CESR 6.0 GeV 100 mA

$\epsilon_x = 50\ nm \cdot rad$ $\epsilon_y = 1\ nm \cdot rad$

Nd - Fe - B

$\lambda_u = 3.3cm$ 61 periods

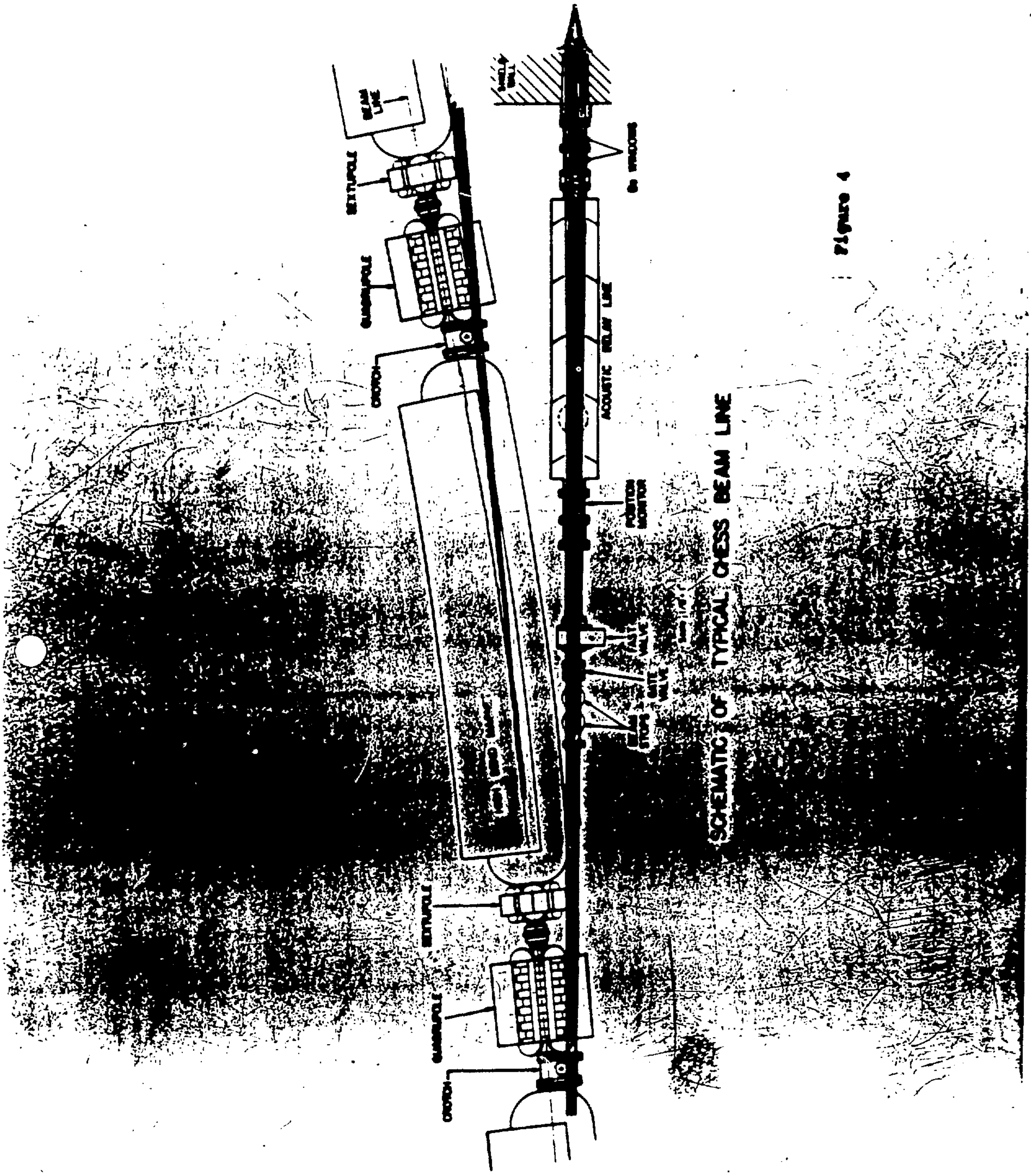
Magnet Gap: 1.35 cm - 2.50 cm

B_o = 5.3 KG — 1.7 kG

K = 1.6 — 0.5

λ_1 = 4.4 keV - 9.1 keV

P_T = 1270 W — 130 W



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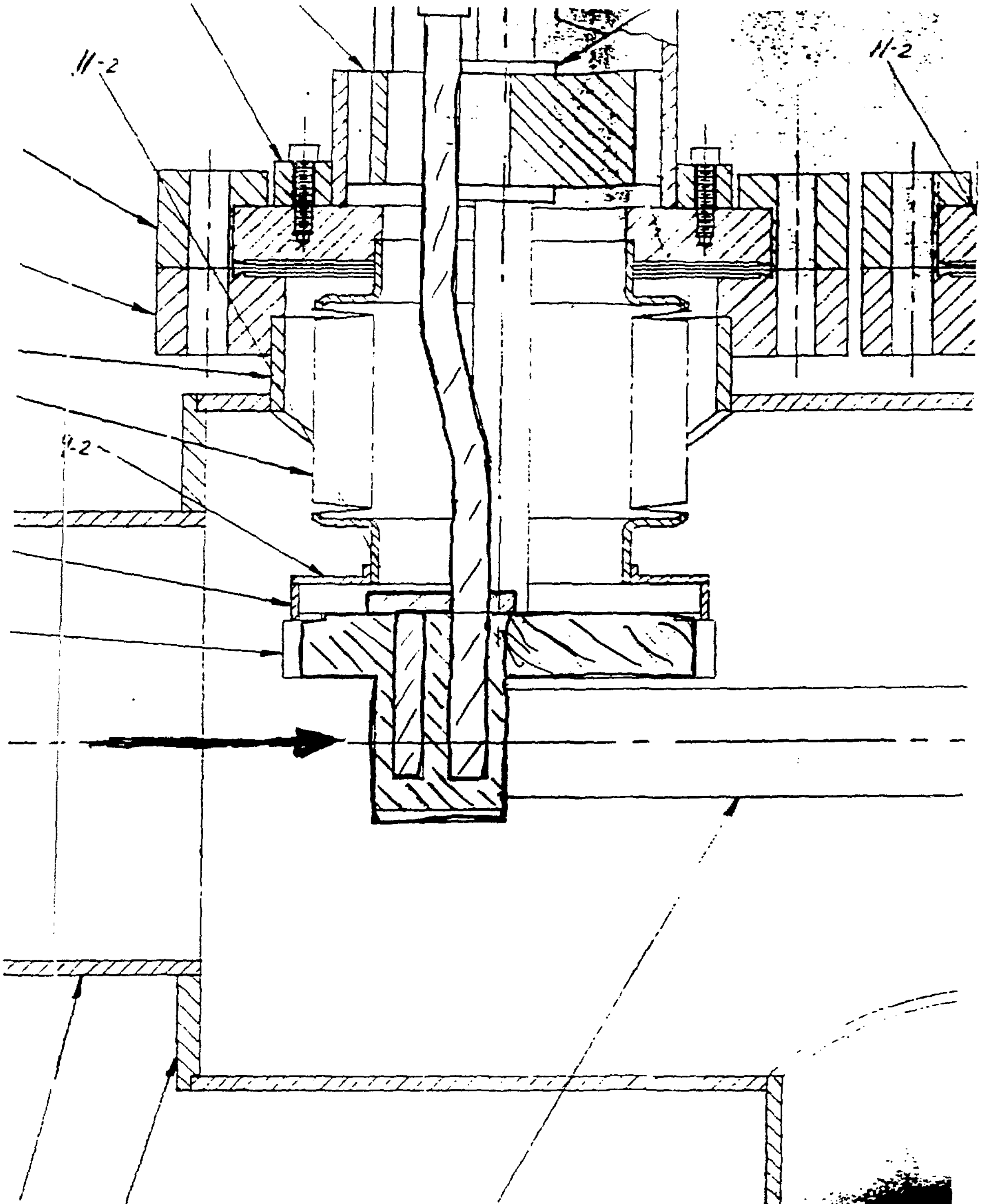
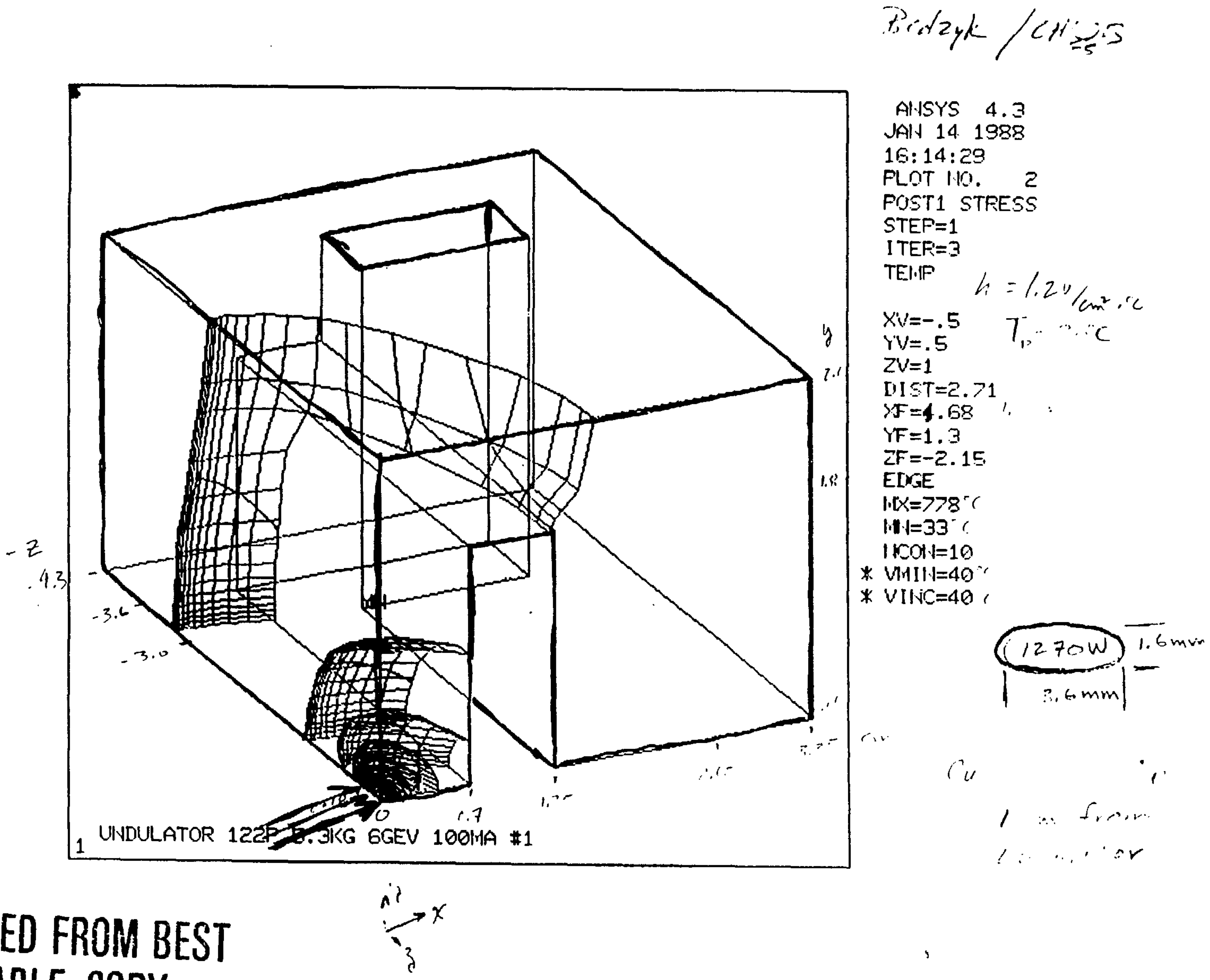


II-2
II-2
II-2



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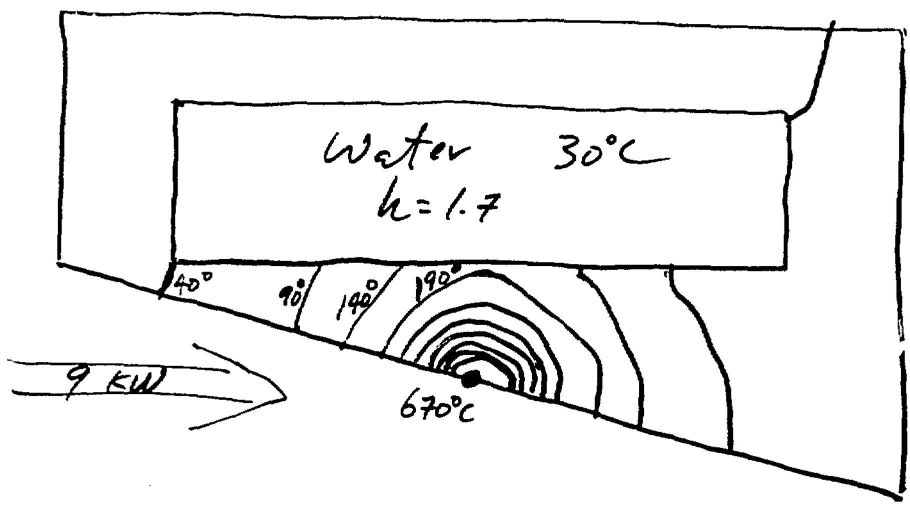
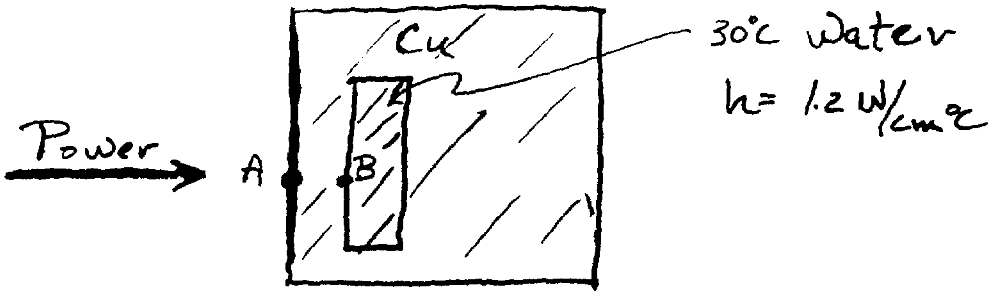
Cu 15° Wedge Beam-Stop



Water Cooled Cu Beam Stop



Heat Load Calculation

6 GeV, 100 mA

	B_o (kG)	P_T (kW)	P (W/mm²)	T_A (°C)	T_B
6P Wig	15	5.1	64	400°	200°
122P Und	5.3	1.3	325	780°	130°
24P Wig	13	9.0	204	1100°	400°

↑ @ 10 m.

R&D EFFORTS AT BNL IN SUPPORT OF THE ADVANCED PHOTON SOURCE*

Peter Stefan
Brookhaven National Laboratory

*The following copies of viewgraphs were provided by the speaker.

R&D EFFORTS AT BNL IN SUPPORT OF THE APS

1. STUDIES OF CRYSTAL COOLING UNDER HIGH POWER LOADS.

2. POSITION MONITOR AND ORBIT FEEDBACK SYSTEMS DEVELOPMENT

3. SMALL-GAP INSERTION DEVICE PROGRAM

4. DESIGN STUDIES OF EXIT CHAMBERS FOR HIGH POWER LOADS

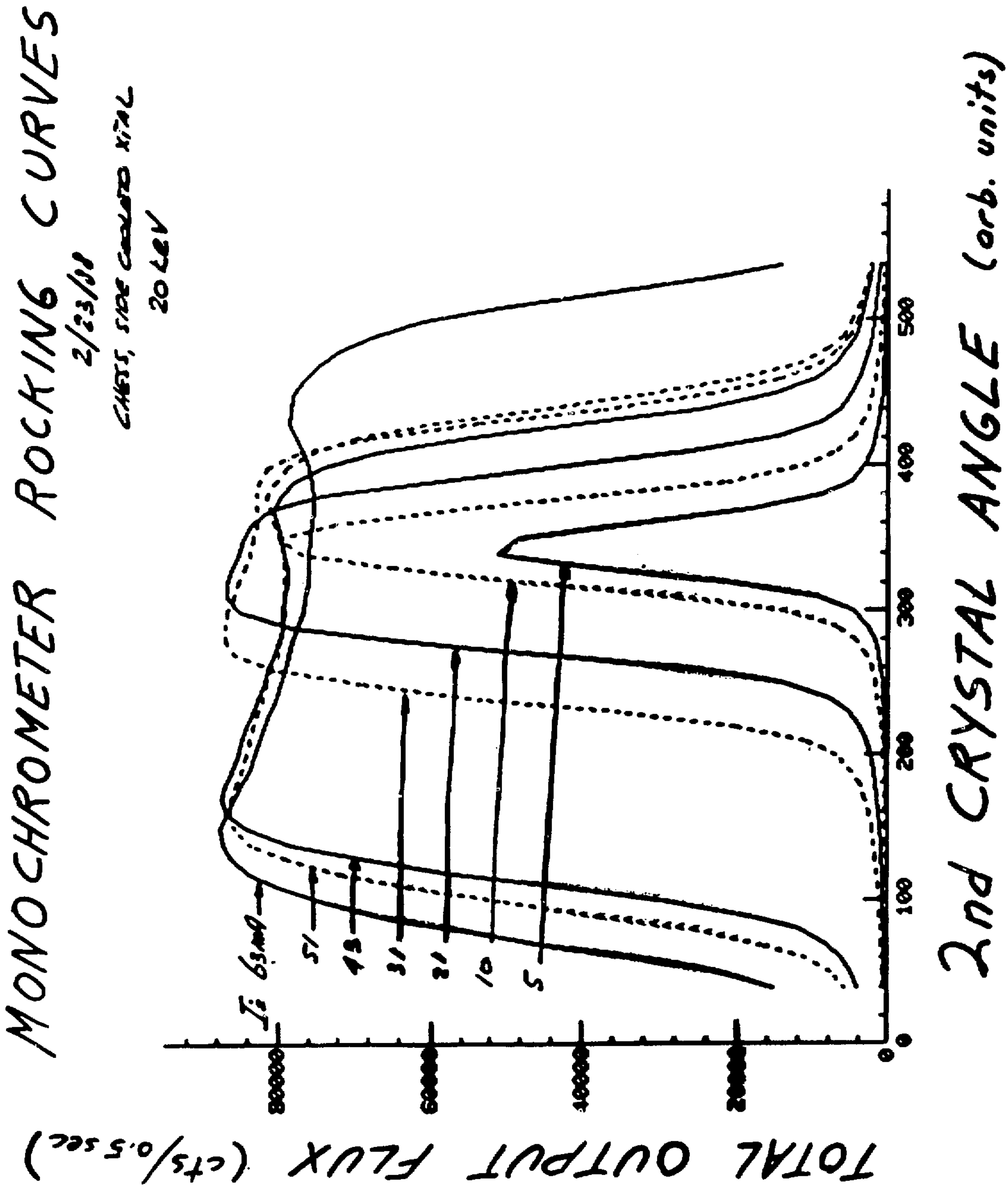
CRYSTAL COOLING
UNDER HIGH POWER LOADS

WORKSHOPS AND COLLABORATIVE EFFORTS INVOLVING:

ANL, BNL, CHESS, EXXON, LBL

PARTICULAR BNL CONTRIBUTIONS:

1. X-25 R&D PROGRAM
2. SAW-CUT CRYSTAL-COOLING SCHEME



MONOCHROMETER ROCKING CURVES
CHESS, SIDE COOLED XTAL
20 keV
TOTAL OUTPUT FLUX (cts/0.5 sec)
2nd CRYSTAL ANGLE (arb. units)
63mA
51
48
31
21
10
5
0
100
200
300
400
500
20000
40000
60000
80000

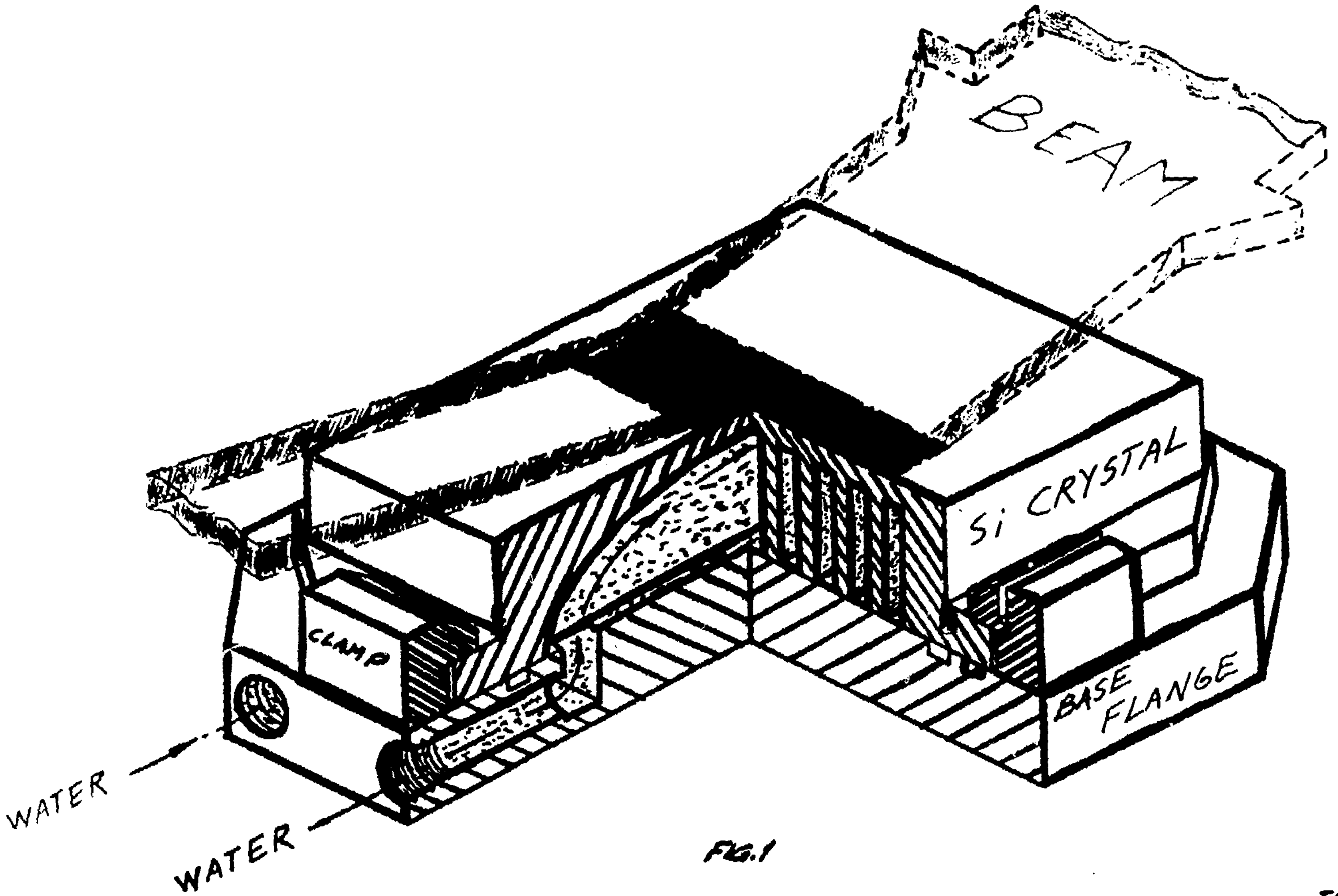


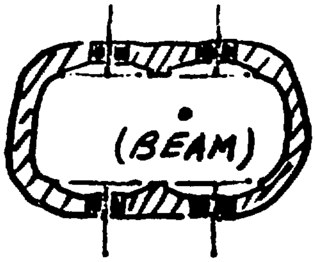
FIG. 1

(TOM OVERSLUIZEN)

T-O-37091

POSITION MONITOR SYSTEMS USING ELECTRON/POSITRON BEAM PICK UP ELECTRODES

(JOHN GALAYDA)



1. SYSTEM FOR ACTIVE-TRIP PROTECTION
   - HIGH DYNAMIC RANGE
   - LOWER SPEED (~100 Hz)
   - LOWER RESOLUTION

2. SYSTEM FOR ORBIT STABILIZATION
   - HIGH RESOLUTION (NSLS "NOISE FLOOR" 2μm)
   - HIGH SPEED (>20 kHz)
   - LOWER DYNAMIC RANGE

HARMONIC FEEDBACK

ORBIT STABILIZATION

(LI-HUA YU)

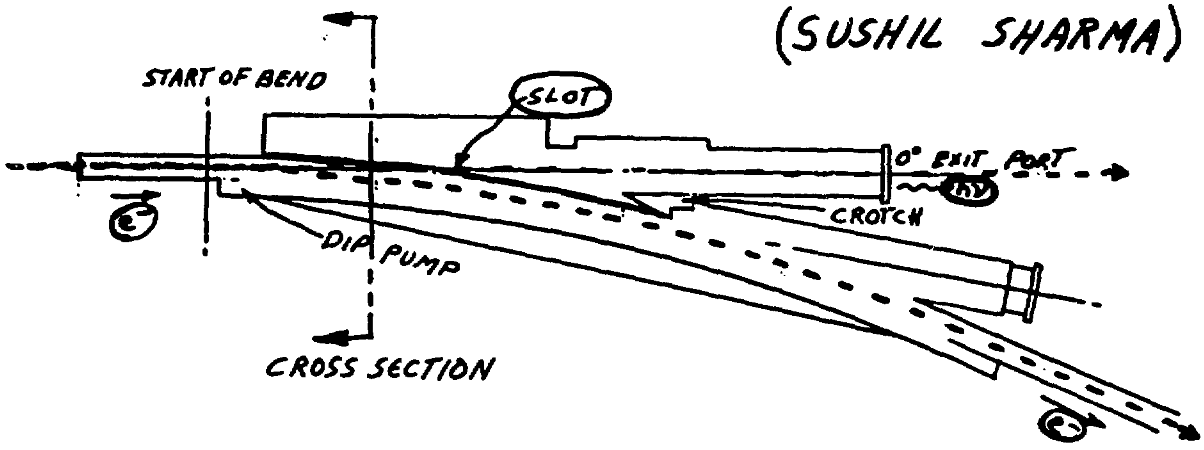
1. PRODUCES A GLOBAL CORRECTION
2. REQUIRES LOW CORRECTOR STRENGTHS
3. MUCH LESS SENSITIVE TO "TUNE" CHANGES

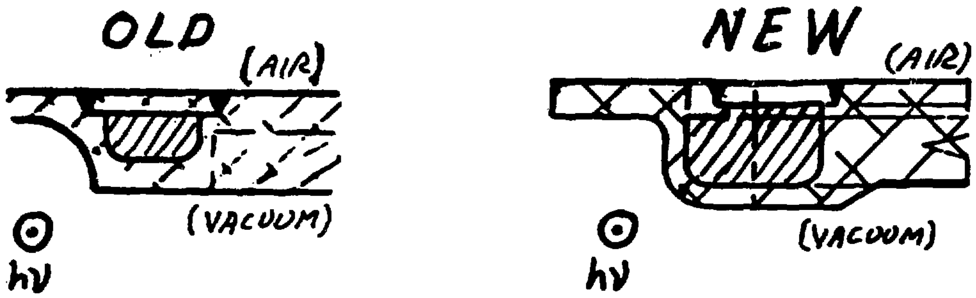
SMALL-GAP INSERTION DEVICE PROGRAM

1. EXPERIMENTALLY DETERMINE THE MINIMUM GAP, AND IDENTIFY THE LIMITING FACTORS.
2. CONSTRUCT AND TEST SMALL-GAP MAGNETIC STRUCTURES.
3. IF WARRANTED, CONSTRUCT A PERMANENT DEVICE AND BEAMLINE.

SLOT MODELING

(SUSHIL SHARMA)





1. MATERIAL CHANGE - 6063 → 2219-T87
2. MOVE WELD FROM CRITICAL AREA
3. ELECTRON-BEAM WELDS
4. DECREASE GRAZING ANGLE - 9° → 6°

~50% IMPROVEMENT IN CURRENT LIMIT.

250mA → 350mA

BUSINESS MEETING OF THE ADVANCED PHOTON SOURCE USERS ORGANIZATION

The annual meeting of the Advanced Photon Source Users Organization was called to order at 11:15 a.m. A set of bylaws proposed for the Organization was adopted (see following page).

Walter Trela summarized the recommendations from the APSUO Steering Committee's review of the APS program, together with the Argonne APS team's response. The Committee had recommended that the shield-wall design be modified to keep the wall as close to the source as possible; this has been done. Previous designs for user laboratory/office modules were not what the users wanted, and the design of these modules has been modified. The expected quality of the experiment area was also improved, in terms of noise control and the ambience on the experiment hall floor.

Trela noted that Argonne was extraordinarily open to user input, giving future users an unprecedented opportunity to have their voices heard. All good suggestions were implemented. It will be the users' responsibility, said Trela, if they are not happy when the APS is finished, because the opportunity existed to be heard. He concluded by thanking David Moncton, Gopal Shenoy, and the other ANL staff for their contributions to the project and the meeting.

The floor was declared open for nominations to fill an opening on the APSUO Steering Committee. (The bylaws adopted earlier provide for half of the Committee to be elected yearly, with two-year terms. It was agreed that the present membership would stand through the present meeting; the nominations were to fill a vacancy.) Those accepting nomination were Howard Birnbaum, University of Illinois; Stephen Durbin, Purdue University; and Stuart Rice, The University of Chicago. The Committee elected Stephen Durbin.

ADVANCED PHOTON SOURCE USERS ORGANIZATION BYLAWS

I. NAME

This organization will be called the Advanced Photon Source Users Organization (APSUO).

II. PURPOSE

The purpose of this Organization is to facilitate the availability and effective use of the Advanced Photon Source by the synchrotron radiation research community so that the greatest overall scientific and technical benefits are realized.

III. ORGANIZATION

Membership - All APS users or potential users are eligible to be voting members.

Meetings - An Annual Meeting of the membership will be held at the APS site. The agenda and brief summaries of discussion items will be posted at the APS and circulated one month in advance of the meeting. The minutes of the meeting will be circulated within two months after the meeting.

Steering Committee - A Steering Committee will be elected to conduct the business of the APSUO. This Steering Committee will consist of 12 members plus the Past Chair. Six members will be elected each year for a two year term. Elections will occur at the Annual Meeting. Interim appointments, if required, will be handled by the Chairman.

Officers - The officers shall be elected by the Steering Committee from its membership for a one year term. The officers of the Organization will be a Chair and a Vice-chair. The Vice-chair will succeed the Chair at the end of the Chair's term. The Chair will remain as an ex-officio member of the committee for the following year. Administrative and financial support will be provided by Argonne National Laboratory.

Officers' terms on the Steering Committee shall be extended as needed to perform the above services.

Steering Committee Meetings - The Steering Committee shall meet at the time of the Annual Meeting and at such other times as called for by the Chair or by a majority of the Steering Committee membership. A quorum consists of a majority of the Steering Committee membership.

IV. FUNCTIONS

The APSUO shall be advisory to the Director of the Advanced Photon Source.

- o The Organization will serve as an advocacy group for the Facility.
- o The Organization will provide advice to the Director on matters affecting the user community.
- o The Organization will assure good communication between the APS user community and the APS management.

V. AMENDMENTS

These bylaws shall be amended by a favorable vote of two-thirds of the members participating in the business part of an Annual Meeting.

Adopted: Walter Trela

DISCUSSION OF APS USER ACCESS POLICY

Jerome Cohen (Northwestern University) started the discussion, noting that the users organization for the APS project was started in the Midwest 5½ years ago. This is only the second meeting of the present organization. Cohen said that Katherine Cantwell chairs the Steering Committee's subcommittee on user access policy. This summer, the subcommittee will transmit a letter to Argonne advising it of proposed policies, and in September 1988 the question of user access policy will be taken up by the full Steering Committee. The Laboratory management will be asked to come to the next APSUO Steering Committee next spring with a policy.

Cohen said there are two issues: what the user policy should be and how the policy should be reviewed.

Katherine Cantwell (SSRL) presented an overview of a variety of approaches considered by the subcommittee. These approaches, framed in terms of "Cooperative Access Teams" (CATs), were as follows:

- Standard CATs
  - A-CATs -- Investigators cooperating on the basis of a common scientific purpose
  - B-CATs -- Investigators cooperating on the basis of pooled resources
  - C-CATs -- Investigators working without the need for cooperation beyond their own organization ("FAT CATs")
- Supported (S-) CATs -- facility owned and operated; facility owned and user-operated
- Rapid Access to Technology (RAT-) CATs -- beam lines available for fast, short-term access
- Academic CATs -- 50% ANL appointments
- Venture CATs -- Fee-for-service beam-line operations (e.g., "mail-order" EXAFS)
- Mil-CATs -- Classified research

Kantwell said the subcommittee is interested in hearing ideas for other types of access over the next six months.

Michael Knotek (NSLS) said there are two major time periods to consider -- getting established and operations. He listed steps to use in formulating the type of CAT one might fit:

Stage	People and Resources	
1.	Goal setting and funding	Scientific and administrative
2.	Design	Scientific, instrumentation, and engineering
3.	Engineering	Engineering, design, and service
4.	Procurement and fabrication	Industry, shops
5.	Assembly	Technical and engineering resources
6.	Commissioning	Scientific and technical
7.	Operation	Scientific, technical, and administrative

Management of the APS must make sure everything is covered, so that facility users and industry support come on line smoothly. Early planning and close coordination will be necessary.

David Moncton (APS) summarized projected costs of the initial beam-line development plan for the APS. Plans call for setting aside a $40-million "trust fund" for the initial (Phase 1) beam lines. He said the "entry-level" cost for an undulator beam line is expected to exceed $3 million. The APSUO will try to help collaborative teams get started. It is proposed that $20 million from the trust fund be used to complete eight beam lines (project funded and staffed by collaborative teams); this includes the USAR professorships. The remaining $20 million would be used to build various insertion devices and front ends, with collaborative teams paying for downstream components outside the shield wall; this would result in approximately another ten beam lines being made available.

Moncton described the sector-management concept, in which each collaborative team would be responsible for a sector (one insertion-device beam line and one bending-magnet beam line, treated as a unit); the collaborative teams could be of various types. He also said proposals for use of the APS should be based on scientific content, competence of the researchers, a management plan, and periodic reviews.

Boris Batterman (CHESS) said an example of the "S-CAT" exists right now at CHESS, where a small laboratory has total ownership of the beam lines and partial use. He cited an NIH-supported biomedical resource as an example of an S-CAT supported by a third party; this resource exists specifically to promote protein crystallographic research at CHESS. A second, formative S-CAT at CHESS is the National Facility for High-Pressure Research. Batterman has committed half time on one beam line for this facility, which is funded for a combination of geoscience experiments.

Robert Broach (Allied Signal Corp.) noted that most industrial users of NSLS beam lines are operating with multiple (four to seven) partners. Broach discussed CAT concepts with respect to the needs of industry. The kinds of access of interest to industry include wholly owned, shared, V-CATs, RAT-CATs, and general user access. Whooly owned lines offer the greatest ease of use for a company, but they also have the highest capital cost. Sharing beam lines is less costly but harder to manage.

Jerome Cohen concluded the subcommittee's presentation, discussing (1) decisions on allowing collaborators to use equipment and (2) Academic CATs, an approach he hopes Argonne will pursue. With Academic CATs, funding would be provided on a 50/50 basis by the Laboratory and the experimenter's university for a faculty position.

General Discussion

Question: In forming and managing cooperative teams, any group would need access to a bending magnet (BM) beam line. Insertion devices (IDs) and bending magnets are tied together in the scheme outlined here. How would time be split between ID and BM lines? Would separate proposals be needed for the ID and BM beam lines?

Answer: A possible solution would be for the Argonne/APS management to arrange that two or three BM lines would be available to ID teams for preparation; BMs are a valuable resource.

Comment (Joe P.): I suggest we think about the division of labor. What percentage of the facility resources should go into providing advice on design and what percentage into construction of beam lines? On the one hand, it's not advisable for the facility to own every beam line; the other extreme, letting people build whatever they want, is also not the best policy. Careful thought is needed about the facility's role as a coordinator.

Ques. (S. Durbin): This trust fund concept sounds like we're creating a new funding agency, to which one could send proposals instead of to NSF or DOE. How would these proposals be reviewed, and what would be the role of NSF and DOE?

Ans. (Cohen): The trust fund is not intended to serve as a funding agency; it is to be a source of money to help build *some* beam lines.

Ques. (Paul Heiney): With regard to the funding issue, we're talking about 100 beam lines eventually, at about $3 million apiece. Where's the money coming from? There may be some FAT CATs, but a lot of the funding will have to come from DOE and NSF -- are they ready to make that kind of commitment?

Ans. (Cohen): With bottom-driven organizations, good proposals will be funded. Another place to look is *centers* for particular kinds of research -- for instance, Stanford has a center that's funding a beam line.

Ques.: Could the trust fund be considered as a source of matching funds? Will it be expanded later on, or is it a case of being first with the most? Could trust fund money be used to pay part of the cost on joint development efforts for IDs?

Ans. (Cohen): These are already matching funds. As for the chance for expansion, this is a new approach Dave Moncton has worked out to make a sizable chunk of money available; we have to consider carefully how people are chosen, what the selection rate should be.
(D. Moncton): We're talking about $140 million for beam lines, which with two phases give about $80 million. This is perhaps a factor of two greater than at NSLS.

Norm: Longevity of ownership of beam lines, periodic review of proper use of beam lines.

Cohen: In a proposal, high-quality science will enable you to get the funds you need. Don't scrimp -- plan appropriately.

USER SUBGROUP DISCUSSIONS

Meeting participants were invited to take part in user subgroup discussions under various topical headings at a working lunch on Thursday, 10 March. Subgroup topics are listed below:

- Absorption spectroscopies
- Dynamical diffraction
- Earth sciences
- Inelastic scattering
- Macromolecular crystallography
- Magnetic scattering
- Microtomography
- Small angle
- Surface studies
- Topography

Persons interested in the conclusions reached by the various user subgroups should contact the APS User Administrator, Elizabeth Stefanski.

PROGRAM

SECOND USERS MEETING

FOR THE ADVANCED PHOTON SOURCE

March 9-10, 1988
Argonne National Laboratory
Argonne, Illinois
Bldg. 362 Auditorium

Wednesday, March 9, 1988

Morning Session: Status Reports on the Advanced Photon Source

8:15 a.m. Registration and Coffee

9:00 a.m. **Welcoming Remarks**
Alan Schriesheim, Director, Argonne National Laboratory
Congressman Harris Fawell, House Science and Technology Committee
Donald K. Stevens, Associate Director for Basic Energy Sciences, Office of Energy Research, DOE
John Straus, Executive Director, Illinois State Governor's Commission on Science and Technology
Walter Trela, Chairman of the Steering Committee of the APS User Organization

10:00 a.m. **Advanced Photon Source Project Overview**
David Moncton, Interim Director, Advanced Photon Source

10:30 a.m. Break

CHAIRMAN Walter J. Trela, Los Alamos National Laboratory

11:00 a.m. **APS Accelerator Design**
Yang Cho, Associate Division Director, Advanced Photon Source

11:30 a.m. **Energy and Time Structure of Photons from the APS Insertion Devices**
Gopal Shenoy, Associate Division Director, Advanced Photon Source

12:00 noon **APS Conventional Facilities Overview**
Martin Knott, Advanced Photon Source

12:30 p.m. No-host Lunch, Argonne Cafeteria,
Bus transportation from Bldg. 362

1:45 p.m. Buses return to Bldg. 362

Afternoon Session: Frontiers in Synchrotron Applications
CHAIRMAN: Paul M. Horn, IBM T.J. Watson Laboratory

2:00 p.m. **Millisecond-Resolution Scattering Studies of Phase Transition Kinetics**
Brian Stephenson, IBM T.J. Watson Lab, Yorktown Heights, N.Y.

2:30 p.m. **Synchrotron X-Ray Microtomography**
Kevin D'Amico, Exxon Research and Development, Annandale, N.J.

3:00 p.m. **Liquid and Solid Surfaces**
Peter Pershan, Harvard University, Cambridge, Mass.

3:30 p.m. **Time-Resolved Macromolecular Crystallography**
Keith Moffat, Cornell University, Ithaca, N.Y.

4:00 p.m. **Tour of the Mock-Up of the APS Storage-Ring Sector and Laboratory Reception**

5:30 p.m. Board Buses for Chicago Museum of Science and Industry

6:30 p.m. Cocktails and Dinner at the Museum Sponsored by the University of Chicago
After dinner speaker: Kazutake Kohra, Executive Director, Foundation for Promotion of High Energy Accelerator Science

10:00 p.m. Buses return to Willowbrook Holiday Inn and Argonne

Thursday, March 10, 1988

Morning Session: APS Workshop Reports and User Activities
CHAIRMAN: David Lynch, Ames Laboratory

8:30 a.m. **X-Ray and Neutron Scattering from Magnetic Materials,** November 6-7, 1987, Doon Gibbs, Brookhaven National Laboratory, Upton, N.Y.

8:50 a.m. **X-Ray Synchrotrons and the Development of New Materials,** December 10-11, 1987, Stephen Durbin, Purdue University, West Lafayette, Ind.

9:10 a.m. **X-Ray Synchrotrons and New Opportunities in the Earth Sciences,** January 18-20, 1988, Joseph Smith, University of Chicago, Chicago, Ill.

9:30 a.m. **Time-Resolved Studies and Ultrafast Detectors,** January 25-26, 1988, Paul Sigler, University of Chicago, Chicago, Ill.

9:50 a.m. **Reports on R&D at other Synchrotron Facilities in Support of the APS**

10:45 a.m. Break

CHAIRMAN: Walter J. Trela, Los Alamos National Laboratory

11:15 a.m. **APSUO Business Meeting/Report of APSUO Steering Committee**

11:30 a.m. **Election of New Steering Committee Member**

11:40 a.m. **Discussion on APS User Access Policy**

12:40 p.m. No-host **Working Lunch of User Subgroups** at the Cafeteria, Bus transportation from Bldg. 362

2:00 p.m. Buses return to Bldg. 362

2:30 p.m. Bus departs for O'Hare Airport

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