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Using a 6-GeV Synchrotron Source

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**Research in Atomic and Applied Physics  
Using a 6-GeV Synchrotron Source\***

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**ABSTRACT**

The Division of Atomic and Applied Physics in the Department of Applied Science at Brookhaven National Laboratory conducts a broad program of research using ion beams and synchrotron radiation for experiments in atomic physics and nuclear analytical techniques and applications. Many of the experiments would benefit greatly from the use of high energy, high intensity photon beams from a 6-GeV synchrotron source. A survey of some of the specific scientific possibilities is presented.

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## I. INTRODUCTION

The Division of Atomic and Applied Physics (DAAP) in the Department of Applied Science at Brookhaven is investigating topics in atomic, nuclear, and applied physics techniques, and their applications to other scientific fields. In addition to work in basic atomic physics and the development of nuclear analytical techniques, complementary experiments using ion and photon beams are under way in geochemistry, cosmochemistry, biology, medicine, and materials science. The availability of a Six-GeV Synchrotron Source (SGSS) which can furnish photons with higher energies and higher intensities will be extremely useful for extending the range of experiments which can be undertaken.

The ways that the SGSS can be used and the types of science that will be made possible are outlined in this short report. Great detail in the discussion is not possible because of the diversity of the topics considered. The material covered is the result of efforts by a large number of scientists in DAAP, other BNL departments, and universities. Individuals connected with specific efforts are listed in the discussions of individual topics.

## II. ATOMIC PHYSICS

To date most applications of synchrotron radiation to atomic and molecular physics experiments have concentrated on examination of the loosely-bound outer shells. The use of higher energy radiation available at the National Synchrotron Light Source (NSLS) x-ray ring now makes it possible to devise experiments which probe more deeply

into the atomic inner shells. The SGSS with photon energies to 100 keV allows photoionization of the K-shell of elements to lead and beyond, even with bending magnet radiation, thus opening up a detailed shell-by-shell probe of the atom. Wigglers and undulators to increase photon flux will be necessary in many cases because the required use of low-density targets results in experiments that have very low interaction rates.

High-energy synchrotron radiation for atomic physics has not been widely discussed, and therefore, justification for using the SGSS for experiments of this type will be explored here. Atomic physics is an important field in modern science because there are many basic questions still open in atomic structure and spectroscopy which need to be examined experimentally and theoretically. Particular applications of synchrotron radiation to atomic-physics research were discussed in a 1980 workshop on "Atomic Physics at the National Synchrotron Light Source" [1]. The summary of this workshop is still relevant and is given here as Appendix I<sup>\*</sup> since it gives a succinct summary of reasons for doing atomic physics at the NSLS or at the SGSS.

Atomic physics is also important because it serves as a fundamental building block for other sciences. For example, the results of atomic-physics research are needed for applications in astrophysics, plasma physics, surface science, chemistry, biology, and medicine. These are only a few of the areas where work in the basic science or in the border regions between disciplines will be exciting and rewarding. Some of these points have been detailed in a recent

\* Appendix I removed-cycled separately.  
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workshop on "Current Trends in Atomic Spectroscopy" [2]. Tables 1 and 2 from [2] are given in Appendix 2 to show the usefulness of atomic physics to other sciences and to society.

#### Photoionization Spectroscopy

The simplest type of SGSS atomic physics experiment is the examination of fluorescent radiation resulting from the photoionization of an inner shell in a neutral atom contained in a gas or vapor target. In order to observe noninteracting free atomic systems, a low target density is mandatory and the use of low-efficiency spectrometers is made difficult. Because multiple ionization processes result from the production of a single inner-shell vacancy due to Auger cascades, highly-charged ions can be produced by a single photoionization event. The use of an undulator which produces radiation in the 20-keV region would be ideal for this application. Beam pulse widths in the ps region are necessary for the most versatile experiments that would also use time-resolved spectroscopy to measure lifetimes of the various states involved.

A more versatile way to study the structure of highly-charged ions is the selective photoexcitation or photoionization of ions. The SGSS when combined with the use of ion traps, sophisticated multiply-charged ion sources and heavy-ion storage rings will allow for the opportunity to do precision experiments on almost any element in any charge state.

#### Photon Beam Ion Source

One promising concept is the use of "white light" to successively photoionize trapped ions. DAAP and collaborators are working on the

development of suitable ion-trapping techniques at the NSLS. The production of multiply-charged ions by repetitive photoionization of trapped ions has been discussed by Jones et al.[3], Church et al.[4], and Johnson et al.[5]. Jones et al.[3] showed that it may be feasible to obtain ions such as lead stripped to the K shell with this technique which is called PHOBIS for PHOton Beam Ion Source. A high brilliance source such as the SGSS using undulators or wigglers with appropriate focussing optics could concentrate large numbers of photons in a very small target volume. This would be ideal for PHOBIS which could be used, for example, to study the time evolution of charge states in an argon target as indicated in Fig. 1.

PHOBIS should serve as the basis for an extensive program on the spectroscopy of highly-ionized atoms. PHOBIS can also be a source of low-energy multiply-charged ions that can be extracted, formed into a beam, and used for experiments which study ion-atom interactions in a very general way at energies in the eV range.

For molecular-physics studies, traps could also be used to study the evolution of binding energies as the target is varied from a single atom to a multi-atom cluster. It could therefore be possible for the first time to follow step-by-step the change from atomic energy levels into those appropriate for small clusters, and then into ones that will approximate surface layers or bulk materials.

Another approach to the study of ionized species will be the use of ion beams produced by EBIS (electron beam ion source) or ECRIS (electron cyclotron resonance ion source) techniques. These sources are now starting to produce large beams of highly ionized atoms which

may be of sufficient intensity to be useful for crossed beam experiments. The ion energies are higher than those from PHOBIS which is less suitable for ion-atom experiments, but the currents will be greater which is more desirable for ion-photon experiments. Use of these sources combined with bunching techniques and high brilliance photon sources make possible the consideration of crossed beam experiments that can be done on a very extensive collection of ionized elements. The luminosities for several types of experimental configurations have been listed by Jones et al.[3] and are sufficient in many cases to do sophisticated spectroscopic experiments. The ability to make systematic measurements on nonclosed shell atoms will be of great interest and help in the development of the field.

#### Ion-Photon Interactions

There will be many cases where the intensity of ion beams produced by the basic ion source is not sufficient for crossed beam experiments. For the most versatile solution to this problem, DAAF has proposed [6] that a heavy-ion storage ring be built at the NSLS. The concept of coupled electron storage ring and heavy-ion storage ring to optimize photon-ion interaction rates is called APIPIS for Atomic Physics Ion-Photon Interaction System.

The use of heavy-ion storage rings coupled to ion sources of various types is a concept that has been much discussed [7]. Rings at Stockholm, Heidelberg, and GSI have been funded, and construction has started. These rings will be used for different types of atomic physics experiments including crossed beam work with other ion beams, electron beams, and laser beams. The great virtue of these devices is

that they should be able to store highly charged ions in quantities from  $10^8$  to  $10^{11}$  depending on the ions and the limitations which are inherent in the ring physics. Since they operate at energies of the order of 10 MeV/u the effective beam current corresponds to the orbital frequency times the number of ions in the ring. The prospective currents are then in the mA region which is perfectly adequate for crossed beam experiments with electrons, lasers, or photons from a storage ring.

The heavy-ion storage ring will be very useful at the SGSS when coupled either to an undulator or wiggler. The ideal situation would be to arrange the ring in such a way that access to either type of radiation is possible. The wiggler is needed to ionize K shells of the heaviest elements. The higher brilliance of the undulator at 20 keV would have its own advantages for experiments with other shells. Use of beams of electrons and ions, or laser photons, would be used to make this an extensive facility for atomic physics research that could be used in different ways for experiments with the SGSS or as a stand-alone facility. DAAP hopes that it will be possible to construct the first APIPIS at the NSLS. The scope of the possible experiments is so large, however, that the concept is worthy of consideration for the SGSS, even if one system is in operation at the NSLS. A layout of a possible APIPIS ring at the NSLS is shown in Fig. 2 to give an idea of the amount of floor space required for installation.

The DAAP atomic-physics work is being undertaken by: K. W. Jones, B. M. Johnson, and M. Meron (BNL) in collaboration on various



aspects of the work with V. Kostroun (Cornell), T. H. Kruse (Rutgers), D. A. Church (Texas A and M), and I. A. Sellin (Tennessee).

### III. ANALYTICAL TECHNIQUES

The development and improvement of analytical techniques and methods using radiation from the SGSS should bring about major improvements in the characterization of materials and as a result lead to many new areas of research in various scientific fields. DAAP and collaborators have explored some questions relating to this field in earlier experiments at the Cornell University CHESS facility and are currently working at the NSLS. From this experience several simple concepts emerge which will be important, in our opinion, to develop and exploit at the SGSS.

The techniques that are of interest will include x-ray optics for producing high flux beams and improvements to synchrotron radiation-induced x-ray emission (SRIXE) used for trace element detection and to various methods such as EXAFS, XPS, etc. that can be used for chemical speciation.

The most important single need is the provision of a high brightness source that will maximize the flux of photons at the sample position. The size of the spot required will be dependent on the type of work to be done. It will not necessarily be true that only very small spots are usable.

The ultimate goal is to push the minimum detectable limits (MDLs) in bulk solid, liquid, or gas samples as low as possible. Early experiments and calculations show that it should be possible to get

MDLs which are 10-100 parts per billion (ppb) by weight. If a higher photon flux of appropriate energy can be attained with an undulator or wiggler, then attempts to push these levels lower should be rewarding. Measurements on small liquid samples below the ppb level start to extend what can be done with inductively-coupled plasma spectroscopy (ICP) and to the same regime as mass spectrometry (MS). Differences in sample sizes and preparations in the various methods would probably assure that they would be mutually useful. Alternate methods for standardization of concentrations would also be helpful. It should be emphasized that the problems of sample preparation and contamination at the ppb-level are absolutely monumental. The SGSS infrastructure must, therefore, have state-of-the-art clean room and sample preparation facilities. Complementary characterization facilities such as electron microscopy, AES, SIMS, and ion beam analysis capabilities should be integrated into the system.

Smaller spot sizes are of importance in the analysis of bulk samples when a wavelength-dispersive spectrometer (WDS) is used rather than an energy-dispersive spectrometer (EDS). The WDS is important for resolution of x-ray interferences and in the high-resolution measurements used for chemical speciation. This type of work could benefit from the use of a focussed x-ray beam that has a size of some tens of micrometers.

In the limit, a spot size as small as possible is applicable to making measurements on the very small structures that are of interest in many fields. There is, however, no sharp threshold as to where a x-ray microprobe would be of interest. Rather, there is a continuum

of structures and problems to investigate which assure that any improvements in the analytical technology will be taken and used very quickly.

DAAP is working on various aspects of the x-ray microprobe technology, as are other groups around the world. Projects involving x-ray focussing and x-ray pinhole collimators are in progress. It is now thought that there will be strong limitations to the ultimate progress that will be possible with these approaches and that it will be necessary to start work on alternative methods such as the use of position-sensitive detectors, exposure of photoresists, pinhole cameras, and more sophisticated image processing techniques to fully exploit the potentialities of the SGSS or NSLS for refined materials characterization.

Finally, another technique that will be of great importance in the development of the field will be the increased use of computerized microtomography (CMT). Several groups have demonstrated good results with tube-produced x rays. Recently, work has started at the NSLS by P. Boisseau and L. Grodzins (MIT) and P. Spanne (Linköping and DAAP). There will be many applications of the technique on samples ranging from the micro- to macro-scale, and CMT should be invaluable as a result. The versatility of the SGSS and NSLS as photon sources will ensure that CMT can be used to best advantage.

DAAP projects on analytical techniques are carried on by K. W. Jones, B. M. Gordon, and A. L. Hanson. The development of the microprobe is in collaboration with J. Hastings (NSLS), M. Howells (LBL), J. V. Smith, M. L. Rivers, and S. R. Sutton (Chicago). The

DAAP CMT work is in collaboration with C. Carlsson and P. Spanne (Linköping).

#### IV. BIOMEDICAL RESEARCH

Biomedical research covers a large number of disciplines which have diverse needs for analytical techniques. In some cases extremely sensitive analysis of small samples is necessary, but good spatial resolution is not particularly needed. In other instances spatial resolution and detection sensitivity are important. The spatial resolution of interest will depend on the problem and could well vary from values of the order of 100 micrometers or more to cellular dimensions of 10 micrometers or less. The choice of optimum photon energy also will depend on the situation. The measurement of transition elements in thin samples is best done with moderate energy photons. CMT of humans or the in-vivo measurement of lead in the tibia requires an energy up to 100 keV. The needs of biomedical research, therefore, will best be satisfied by a versatile photon source.

The application of x-ray microprobe methodology has enormous potential to make lasting and significant contributions to understanding the role of essential toxic trace elements in biological systems. Biological organs and tissues are structurally complex and functionally and biochemically heterogeneous at a microscopic scale. The x-ray microprobe provides multielemental localization at the near cellular level, thus permitting a more sensitive and exacting correlation of trace element localization with the structural and

functional organization of tissues and organs. This approach has wide applications in the biochemistry, metabolism, physiology, nutrition, pathology, and toxicology of trace elements which are currently underway in DAAP.

DAAP is working on the application of SRIXE to varied problems in trace element biology and toxicology. The experiments need the simultaneous detection of heavy metals such as cadmium and lead and the usual essential trace or minor elements such as iron, copper, zinc, calcium, potassium, phosphorous, and sodium. Relatively high energies are needed to fluoresce cadmium and lead compared to the lighter elements. The interactions between these elements demand that it be possible to produce lower energy photons at times to study the light elements with low backgrounds. The availability of a tunable source with sufficient intensity to make possible the use of WDS with small spot sizes (10 micrometers) to produce elemental maps of cells or thin tissue sections would represent a major step forward in biological trace element measurements.

#### Lead-Calcium Interactions

Lead is a ubiquitous environmental toxicant with diverse and insidious toxic manifestations. The complex interactions between local and many essential elements, primarily calcium, iron, zinc, and copper, have been reported in experimental and clinical studies. The mechanisms and biological significance of these interactions are not clearly understood. The high sensitivity, good spatial resolution, and multielemental analytical capabilities at the DAAP microprobe are currently being applied to this important problem.

### Ultratrace Essential Elements

The last few years have seen considerable activity in the identification of "new" essential, ultratrace elements and understanding their biochemical function. Molybdenum, selenium, chromium, nickel, vanadium, silicon, and arsenic are considered essential for normal biological function, but in many cases the specific biochemical function(s) is not known. The DAAP has a continuing research activity involving the localization of trace elements in brain structures. PIXE and SRIXE are currently used to investigate the role of essential and toxic element nutrition in the microscopic localization of trace elements in the mammalian brain. The SGSS would greatly improve our sensitivity for these important trace elements.

### Protein Binding

Many, if not most, enzymes require one or more trace elements for structural integrity and/or catalytic function. Electrophoresis provides for the separation of proteins based on their physical characteristics. An important biomedical application of SR is the combined use of SRIXE and protein electrophoresis to provide a sensitive quantitative, multielemental "stain" for electrophoresis gels. This approach is a very powerful research tool (theoretically) for investigating the gene regulation, cellular and molecular biology of many important proteins.

### In Vivo Measurements

At SGSS energies there will be many applications for making in-vivo fluorescence measurements and using CMT to make

high-resolution maps of organs that cannot be done with conventional computerized tomography. DAAP is also engaged in several projects of this nature.

A very sensitive measurement of the amount of lead stored in bone will have great value as a diagnostic tool. This is because it is now becoming apparent that lead has major public health effects that concern a large fraction of the population. In addition to well-known evidence that it can produce neurological defects, learning disabilities, and growth retardation in children, there is an accumulation of evidence which shows it may cause kidney damage, hypertension, heart disease, and stroke as well. The damage is caused by a long-term integrated exposure and hence cannot be assessed by use of blood-lead determinations, but can be measured by use of a noninvasive x-ray fluorescence measurement.

DAAP has worked for several years on the use of  $^{109}\text{Cd}$  88-keV gamma rays for fluorescence of the lead K-x rays in the tibia. It is possible to find lead at the level of about 10 ppm wet weight. Since the known concentrations in the normal population, children and adult, will start below this level, greater sensitivity is essential to have. For use in hospitals or mobile units the use of hotter sources will help. For research purposes the use of synchrotron radiation will make possible great improvements in the measurements through the better angular collimation, higher source intensity, better spatial resolution, and high degree of polarization which will reduce the intensity of Compton-scattered x rays. A project of major medical significance can be mounted using either a wiggler at the NSLS or

bending magnet source at the SGSS and equipped to handle patients brought to the facility for diagnostic and research purposes.

Computerized Microtomography (CMT)

The use of CMT has tremendous potential when coupled to the use of high energy photons which can traverse major biological objects of the size of the human skull or thorax. The in-vivo noninvasive measurements which will be made possible should also have large number of uses for diagnostic measurements and research work. A facility able to process numbers of patients must be associated with CMT. Spatial resolutions with CMT should be 1 mm or less for the in-vivo measurements, and this capability will represent a great improvement in diagnostic capabilities. It should be of interest to list a few topics which concentrate on investigation of the brain.

It may be possible to assess the distribution of atherosclerotic plaques in the cerebral arteries. These are almost always very well demarcated from the "normal" artery in which they are situated. That is, they tend to be within segments of virtually normal artery. Thus, cerebral arterial disease would be visible while it is progressing, before it becomes symptomatic. It would also be possible to noninvasively study and diagnose other small features such as small berry aneurysms of the cerebral arteries, small cysts which obstruct the third ventricle and small tumors of the pituitary. The assessment could be done noninvasively, and the effect of therapy and diet for high-risk patients could be studied. These are examples of the improvement in neurological diagnosis in-vivo that could result from the excellent detail in images of the human central nervous system that will be produced using SGSS CMT.



DAAP work in biomedical research is done by the scientists listed under analytical techniques in Section III above. The CMT work is the particular province of P. Spanne and his colleagues from Linköping University for the hardware and of D. N. Slatkin of the BNL Medical Department for the possible applications. R. Beeuwkes of Smith Kline & French has stimulated many of the thoughts on measurements of light elements and applications of SRIXE to problems in bulk analysis.

#### V. TRACE ELEMENT GEOCHEMISTRY AND COSMOCHEMISTRY

The application of SRIXE to problems in trace element geochemistry and cosmochemistry will be of great importance because of the unique features of the method. In particular, the SCSS would permit very sensitive determinations of the rare earth elements (REE) which require photons up to 90 keV for K-shell excitation.

Many specimens of interest are small (down to a few microns), isolated grains not demanding high spatial resolution. Conventional petrologic thin section require a microbeam with dimensions to the neighborhood of ten microns or less. The availability of a precise CMT capability will be an asset in studying the homogeneity of samples. Rapid production of x-ray maps similar to those produced with the electron microprobe, but with lower MDLs, will bring a unique and entirely new capability to experimental geochemistry and cosmochemistry.

The use of high-energy synchrotron radiation from the SCSS or from a wiggler at the NSLS will open many new types of experiments.

To illustrate the strength of the scientific case that can be made, some particular experiments are described below.

### Sulfides

Trace element analyses for platinum group elements at the micrometer scale are desired to pinpoint the geochemical behavior of these elements in sulfide-bearing environments. Such information would aid the search for geological sources of these economically important metals [7].

### Silica Minerals

The color, luminescence and strength of silica minerals is controlled to a large extent by trace contents of impurities which in turn relate to geological provenance. In principle, trace element signatures provide a means of deducing the primary source of the mineral constituents in a rock. Applications to Archaen geology are particularly desirable to unravel the complex history of the Earth's early crust.

### Sediments

Knowledge of the REE content of sediments would provide valuable insight into their origins. Tephra layers from dated polar ice cores could be characterized, their volcanic sources inferred and ancient volcanic activity studied. Similarly, the geochemistry of specific modern volcanic events could be documented through analyses on particles from plumes and collected in the atmosphere. Geochemical anomalies associated with biological extinctions (e.g., the infamous Ir-enrichment in Cretaceous/Tertiary clay) could be explored.

### Meteorites

REE in meteorites are cosmochemically important because although these elements behave in a roughly analogous manner chemically, they exhibit greatly different degrees of volatility. Relative abundances are therefore sensitive indicators of condensation conditions in the early solar nebula and subsequent metamorphic events. Much interest currently exists in studying the REE contents of calcium- and aluminum-rich inclusions found in carbonaceous chondrites, aggregates which are thought to be some of the earliest condensates [8].

### Cosmic Dust Particles

NASA is currently collecting dust particles (~ 10 micrometers in size) from the upper atmosphere with U-2 aircraft. Many of the particles are clearly extraterrestrial, based on the presence of solar flare tracks, for example, and represent an important source of meteoritic material complementary to the meteorite collection. Circumstantial evidence exists suggesting a cometary origin for the "fluffy aggregate" subset of this material. Trace element analyses of these particles would constrain the identification of their parent bodies and help decipher their histories. The development of analytical techniques for trace element analyses of these small particles would also be important for the eventual study of "comet-return" samples and cosmic material collected in Earth orbit by satellites and/or Space Station [9].

### Tests for Petrogenetic Models

The study of planetary differentiation has important implications for the Earth and other Solar System bodies. Petrogenetic models are

tested by measuring the compositional trends in ultramafic rocks exposed on the Earth's surface and products of laboratory experiments. REE partitioning has proved to be a versatile geochemical indicator in this research [10].

The work in geochemistry and cosmochemistry is being pursued at the NSLS by J. V. Smith, M. L. Rivers, and S. R. Sutton (Chicago) in collaboration with DAAP scientists. Most of this section was prepared by S. R. Sutton.

#### VI. APPLICATIONS IN ARCHAEOMETRY

Applications of SRIXE to archaeometry will be useful. The types of experiments and materials are rather similar to those of interest in the geosciences including trace element fingerprinting. For this reason in this report it will be only mentioned in passing. A summary of possible uses has been given recently by Harbottle et al. [11].

#### VII. SUMMARY

Activities of the Division of Atomic and Applied Physics in the Department of Applied Science at Brookhaven which are relevant to the scientific case for use of insertion devices and the proposed Six-GeV Synchrotron Source are discussed. Some of the experimental requirements for satisfactory pursuit of the work in atomic physics, technique development, and applications are as follows.

1. Several types of sources of photons will be necessary. Use can be made of ordinary arc magnet sources, undulators, and wigglers.

High brilliance sources are necessary for a majority of the applications.

2. In atomic physics the use of ion sources and possible ion storage rings will necessitate substantial space around the target area.

3. White light will be necessary for some of the work.

4. Trace element analyses require extensive ancillary characterization equipment, microscopy facilities, and clean rooms. These needs exist for both biological and geological experiments. Some, but not all, of the equipment can be shared.

5. Separate biological and geological laboratories are necessary for the outside user groups that will come to the facility. There should probably be an in-house program associated with the facilities to ensure that they run properly and to assist outside visitors.

#### ACKNOWLEDGEMENTS

The work described in this summary represents the efforts of the DAAP at BNL and of many outside collaborators. The main contributors are acknowledged above, and apologies are made to anyone inadvertently omitted.

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FIGURE CAPTIONS

- Figure 1. Time evolution of charge states produced by irradiating a Kingdon trap with synchrotron radiation. See Ref. 3 for other details.
- Figure 2. Possible arrangement for APIPIS on a NSLS beam line. The squares represent one meter intervals. The synchrotron storage ring shown is the CRYRING machine to be built at the Institute of Nuclear Physics in Stockholm. The size of the ring is largely dictated by the need for straight sections that contain apparatus needed for experiments and machine operation.

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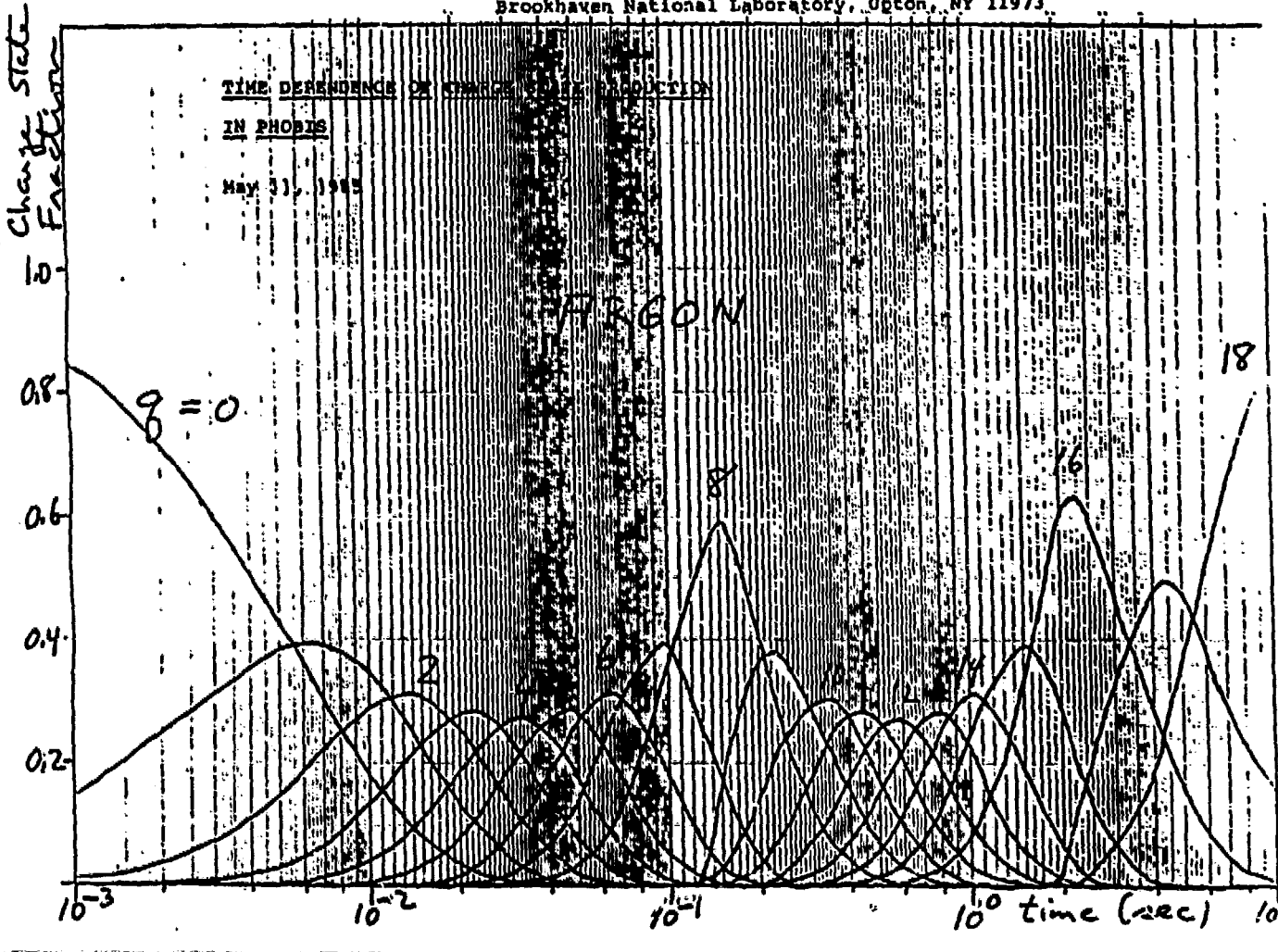


Figure 1



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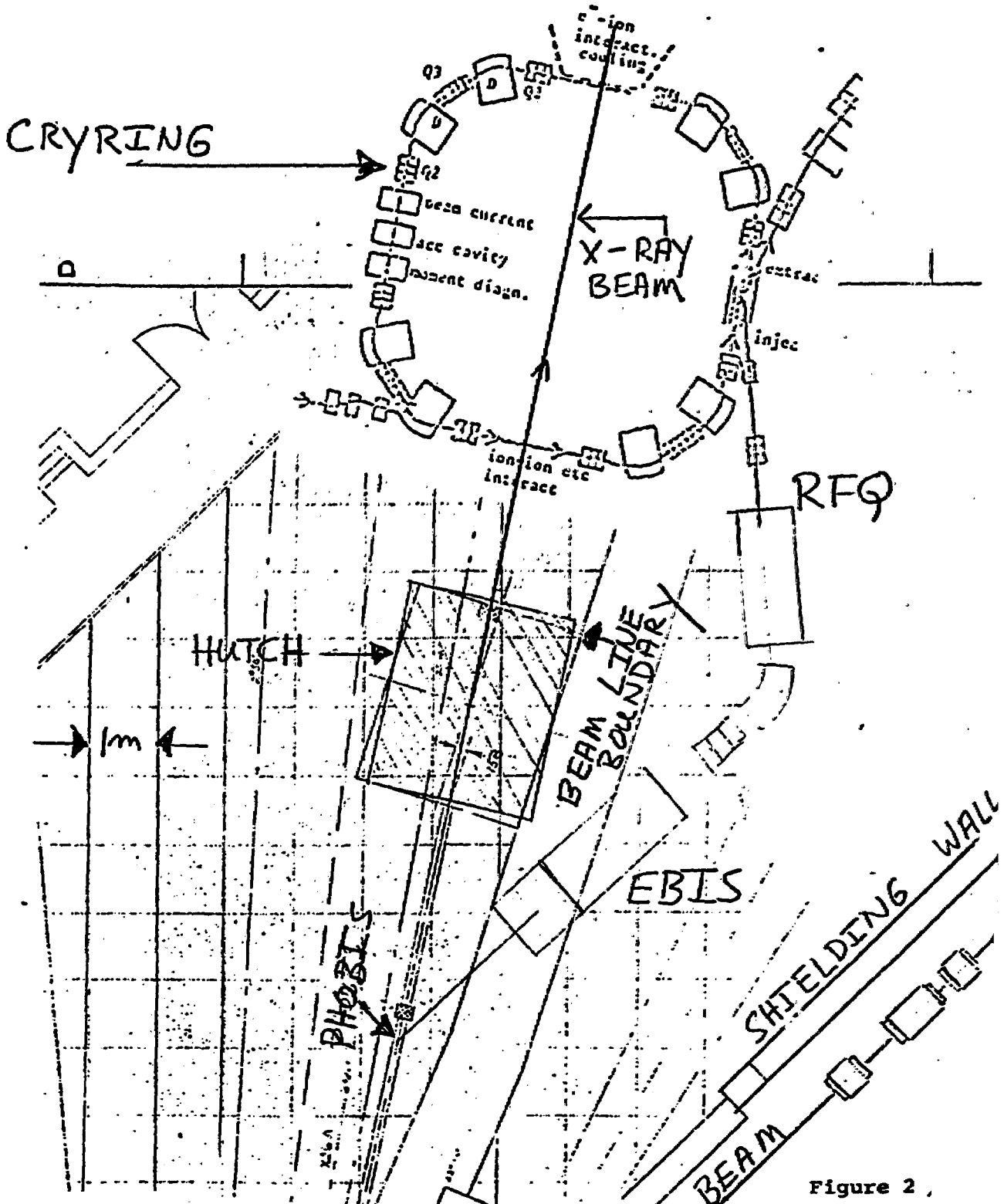


Figure 2