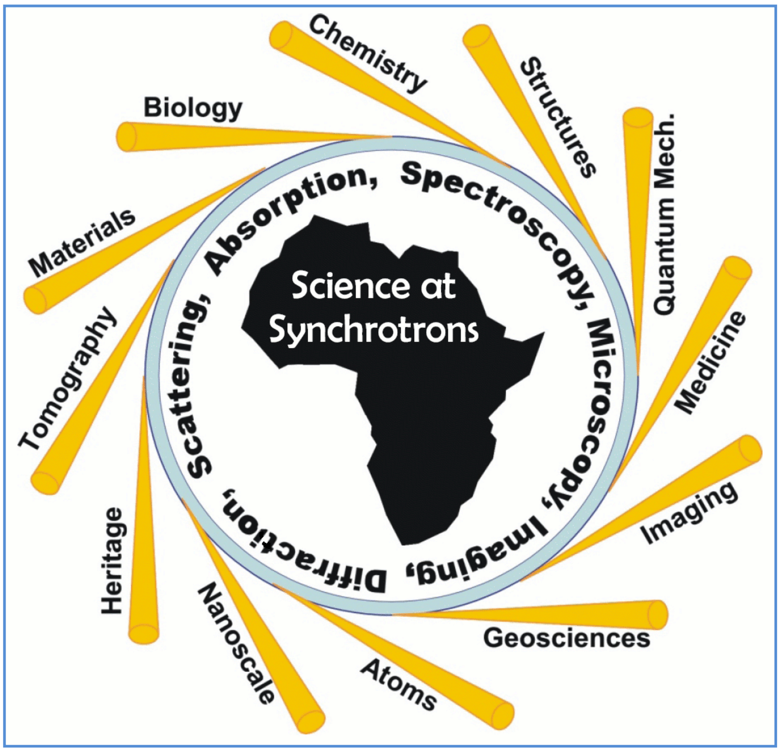
# Feasibility Study for a South African Beamline at an International Synchrotron Radiation Source





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## Preamble

Synchrotron radiation sources are the most powerful modern multi-disciplinary scientific instruments. They are single research tools, able to provide a variety of effective radiation probe techniques to address topical problems in a wide spectrum of disciplines. The high photon flux provided by 3rd generation sources along with major advances in detector technology and data analysis allow significant advances to be made in numerous research fields, and in many cases have resulted in a revolutionary impact. Amongst the disciplines to benefit are materials and nano-science, the life sciences, mining technology, and earth, environmental and heritage sciences. Significant examples include drug development and better understanding of diseases based on protein and viral structures determined at synchrotrons, new models of deep earth dynamics from experiments conducted at pressures approaching those present at the core, and advances in data storage through studies of electronic structure and magnetism. Greater understanding of the properties of materials and processes such as stress and strain now allow new materials with enhanced properties to be developed. Great promise is also being shown in direct medical applications, with innovative imaging techniques, for example of the heart, lung, brain and in mammography, now being complemented by new therapies[1]. More recently the fields of heritage and palaeontology have benefited greatly from, amongst others, the possibility at synchrotrons to generate three-dimensional images of objects such as fossils and bones[2].

There are now close to 60 synchrotron radiation light sources in operation or advanced stages of design and construction around the world[3]. Amongst the list of recently completed third generation light sources are SOLEIL (France), the Australian Synchrotron, the Canadian Light Source, Diamond (UK), and SSRL (USA). Others are in construction in Amman, Jordan; Barcelona, Spain and Shanghai, China. Plans are underway for NSLS II (USA) and the Taiwan Photon Source. The growing importance of synchrotron radiation in an ever widening number of fields can best be summarised by the following statement, from a previous assessment exercise in the USA. This study was completed 10 years ago and the field has grown significantly since then[4]:

"*The most straightforward and most important conclusion of this study is that over the past 20 years in the United States synchrotron radiation research has evolved from an esoteric endeavor practiced by a small number of scientists primarily from the fields of solid state physics and surface science to a mainstream activity which provides essential information in the materials and chemical sciences, the life sciences, molecular environmental science, the geosciences, nascent technology and defense-related research among other fields. The user community at U.S. synchrotron facilities continues to grow exponentially, having reached more than 4000 on-site users annually in FY97. The research carried out at the four D.O.E. synchrotron sources is both very broad and often exceptionally deep.*"

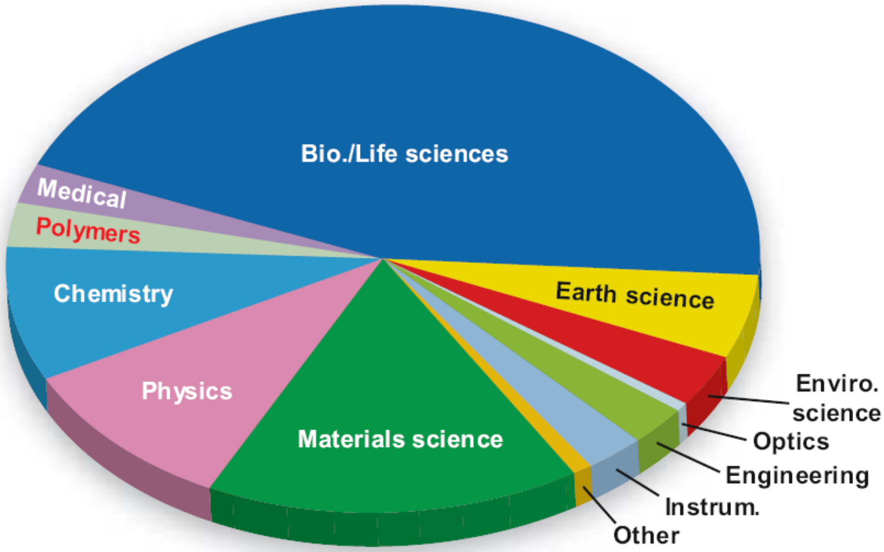


**Figure 1** Distribution of users by research interest at the APS synchrotron (Chicago, USA)[5].

No synchrotron source exists on the African continent. A South African beamline at an already existing synchrotron source would serve as an important step to bridging this divide and greatly expand opportunities for South African scientists to access synchrotron radiation and train them in its use. Designing, building, and commissioning such a beamline would also provide experience essential to the success of a future African light source. The opportunities for graduate students in many disciplines to use synchrotron radiation would increase dramatically, with a resultant strong impact on the development of science and technology in South Africa. The possibilities offered by a South African beamline or a facility in South Africa will also attract senior scientists working abroad (the "African scientific diaspora") to return to a potentially very scientifically enabling environment which is currently lacking.

This document outlines the issues that need to be addressed for such a beamline to become a reality. The choice to build a beamline at an overseas facility was taken by the Australian scientific community in the early 1990's, a comparable case study, given their similar geographical isolation from the scientific centres of North America, Europe and Asia and comparable synchrotron usage (at the moment when they decided to proceed with beamline construction). From about 5 groups using synchrotron radiation regularly when their first overseas beamline was built, they now have about 150 groups a year visiting synchrotron facilities annually. This first beamline is associated by them with a large part of this phenomenal growth which has resulted in their own synchrotron source coming online this year[6]. Many scientists were found to be keener to enter synchrotron science knowing that they would be using what is in effect a national instrument (although based in an overseas laboratory). A South African beamline offers the most direct route to the benefits of synchrotron radiation-based research.

## 1. Introduction to synchrotron-based science[7]

A synchrotron accelerates electrons to extremely high energies and almost to the speed of light. As the electrons are deflected through magnetic fields they create extremely bright light. The light is channelled down beamlines to experimental workstations where matter can be 'seen' at the atomic scale.
Synchrotrons play a pivotal role in research. Synchrotron radiation provides capabilities that are, in many cases, unique and that surpass conventional laboratory sources in intensity, brightness and photon energies by many orders of magnitude. The power of synchrotrons is increasing at a phenomenal rate, exceeding even the rate of development of computer technology.
Synchrotrons are often associated with X-rays, but a synchrotron is not just an X-ray facility. It is an extraordinarily multi-disciplinary research and development (R&D) facility that produces intense light across almost the whole of the electromagnetic radiation spectrum. Using the extremely intense infrared (IR) ultraviolet (UV), soft and hard X-ray, and visible light beams produced at synchrotron facilities, scientists can determine the structure of materials over a huge range of length scales, from macroscopic to atomic levels; study the chemistry of surfaces and interfaces; analyse trace element concentrations in micron-sized samples; measure disordered systems such as catalysts, and amorphous phases in minerals processing contexts; obtain three-dimensional (3D) computed axial tomography (CAT) scan images with micron resolution, and so on. The materials that can be examined range from crystallised proteins and living cells, to hair fibres and mineral deposits, and even to humans and whole animals.

Synchrotron-based research is fast-moving. Research using synchrotron radiation drives progress across the most innovative fields of industry today, including biology and biotechnology, chemistry, physics, electrical and electronic engineering, environmental engineering, mineral exploration and processing, life sciences, materials science and medicine. Synchrotron light has also become an essential tool for investigations in archaeology, palaeontology, geology and many other scientific disciplines.

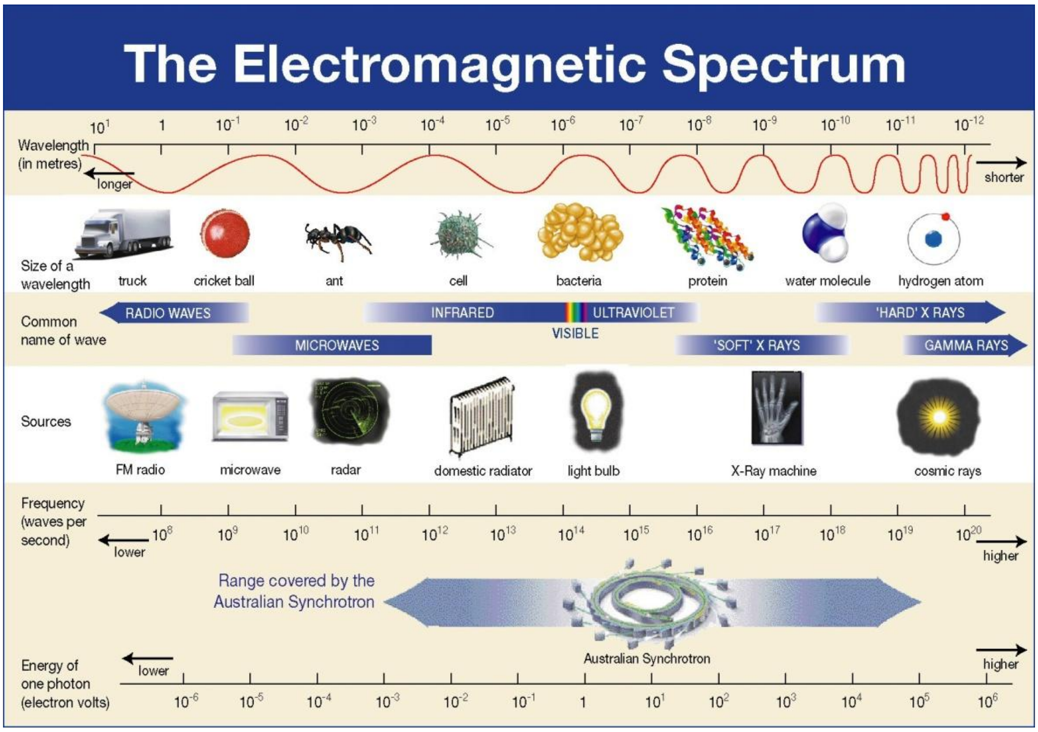


**Figure 2** Figure showing the range of probing radiation in the electromagnetic spectrum that can be derived from, for example, the Australian Synchrotron Radiation source[8].

## 2. Synchrotrons in the context of the National System of Innovation (NSI)

The South African Government has developed the NSI as the guiding framework for major new initiatives in science[9]. A South African beamline at a premier international synchrotron can be shown to deliver massively to the Core Missions and Strategic Priorities of the NSI:

- Core Mission 1: Human resource development
  It will accelerate capacity-building in science and technology because of the level of training, expertise and infrastructure required to operate and maintain such a sophisticated facility. A South African beam-line will serve as a focus and rallying point to boost the development of the local user base and as an international signal of South African intentions and commitment to synchrotron enhanced science capacity. As such a number of South African scientists abroad will be attracted back to the country.

- Core Mission 2: Knowledge Generation (research and development in prioritised areas)
  Much of the research carried out at synchrotrons is at the forefront in its particular field, resulting in a large number of publishable results. As an example, synchrotron experiments conducted at the ESRF yielded 1435 publications in 2006 (Ref. 10). Similarly the beamline will increase the number of publishable results obtained by the South African scientific community. The beamline and the related beamtime sharing agreement will also be tailored to address problems of topical concern to the country. This is further expanded in Section 3 of this report.

- Core Mission 3: Utilisation of research results, technology transfer and innovation
  Industry related projects will have much easier access to synchrotron radiation facilities, with corresponding benefits for the development of new and enabling technologies and

thus the economy. For the construction and upgrades of the beamline new local high-tech industries can be used and if they are not available they can be established, so as to provide some local-content infrastructure at the instrument.

- Core Mission 4: Provision of state-of-the-art-research equipment infrastructure
  Synchrotrons are one of the best examples of state-of-the-art research facilities. The beamline will be one of the flagship instruments of South African science. It will also boost capacity in science and technology at "interface" labs within SA itself because of the level of preparedness required to take advantage of precious beamtime available at an overseas located station.

- Strategic Priority 1: Redress and equity: race and gender
  It is essential that the implementation of every synchrotron-related initiative helps to correct the imbalances that currently exist in South African science. The new opportunities offered by increased access to synchrotron facilities will facilitate this process. The first set of synchrotron meetings held in South Africa was attended by numerous women and people from previously disadvantaged communities (see list of delegates in Ref. 11).

- Strategic Priority 2: Adherence to quality
  Access to the beamline will be controlled by peer-review - see the Section 9 of this report: *Access for users*. This will ensure that only high grade research projects are accepted which in turn will foster a climate of high quality research in the South African scientific community.

- Strategic Priority 3: Internationalisation of research
  Through developing the capabilities of South African scientists and generating an increased number of publishable results of high quality, as outlined in the above points, the beamline will make us significantly increase our international competitiveness in many disciplines.

- Strategic Priority 4: Focus on Africa
  A natural evolution of this beamline and any other synchrotron initiatives is the inclusion of other African countries and their scientists. The human resource development (see Core Mission 1) will then take place in countries in the entire continent. Similarly African scientists working abroad will be attracted to return to the continent. The ability of synchrotron radiation to address local issues and concerns in, for example, biomedical and environmental studies is of particular importance. Some African scientists were already present at the first South African synchrotron workshop (see list of delegates in Ref. 11).

- Strategic Priority 5: Positioning the NRF within the National System of Innovation (NSI)
  The beamline would be classified as a National Research Facility falling under the NRF. As has been shown in this section it will help to consolidate the NRF’s role as an intermediary between science and society.

- Strategic Priority 6: Organisational transformation
  As with all other scientific projects in South Africa the beamline offers an opportunity for the NRF to fulfil the required critical elements in the strategy for its transformation, as outlined in the NSI.

## 3. Beamline characteristics: Matching South Africa's scientific needs

It is of obvious importance to develop a beamline that can best address issues that are of interest to the South African scientific community. However it is equally important to note that, although the beamline would focus on one or two techniques, arrangements can easily be made with the host facility for African scientists to use all beamlines on a priority basis, in return for other scientists to use the African beamline. This has been done with success when beamlines have been built by Australia (at APS and the Photon Factory), and by Brazil at the CAMD light source in Louisiana, USA. There are so many applications of synchrotron radiation, and so many types of specialised beamlines, that it is impossible for one beamline to serve all users. So it is important that such arrangements be made to serve a growing community of users requiring different techniques.

The technique that would appear to be the first choice, both in terms of applicability in a wide range of fields for a single instrument, as well as ease of installation and use, is x-ray diffraction (XRD). An x-ray diffraction beamline offers access to the principal techniques of x-ray (powder and single crystal) diffraction and protein crystallography. The importance and utility of these methods can be seen by the large number of XRD instruments present or under construction at modern synchrotrons. A few examples are: ALBA (Barcelona, Spain): 2 (out of 7); ESRF (Grenoble, France): 12; APS (Chicago, USA): 33; DIAMOND (Oxford, UK): 4 (out of the first 7) plus 3 to be constructed; SOLEIL (Paris, France): 7.

X-ray diffraction allows one to determine the crystal structure of a system, obviously fundamental information for the understanding of its properties. As a result XRD is an essential tool in many fields in which the South African scientific community is active, including materials science, biomedicine, chemistry, geophysics and solid state physics. For example, synchrotron x-ray diffraction is essential to protein structure determination. In turn protein structure determination is vital for the design of medicines, vaccines, agrichemicals and industrial enzymes. One major impediment at present to the growth of structural biology in South Africa is the lack of access to synchrotrons. In the past several years 3 Nobel prizes in chemistry have been awarded based on structural biology work done at synchrotrons, including the 2006 prize to Roger Kornberg for elucidating the structure and function of RNA polymerase. In all cases convenient access to synchrotron radiation sources was critical.

As a complementary technique, and with a minimal addition of instrumentation, the beamline can be easily equipped to perform x-ray absorption spectroscopies (XAS), viz x-ray absorption near edge spectroscopy (XANES) and extended x-ray absorption fine structure spectroscopy (EXAFS). EXAFS is particularly useful in yielding structural information in non-crystalline systems, such as liquids, glasses and nanoscale materials such as carbon nanotubes. XANES, on the other hand, yields information on the electronic structure, of equal importance and complementary to structural studies. Although we have independently arrived at the conclusion that a XRD and XAS beamline is the best initial tool to serve the relatively broad needs of South African research, we would like to note that this was also the same choice made by the fledgling Australian synchrotron community[12]. It is important to note that these techniques require a intense, tuneable photon source and are difficult or impossible to carry out with sources other than a synchrotron.

An important and expanding field of research is the use of XAS in biomolecular research (BioXAS), with particular impact on the study of protein-bound metal complexes (structural genomics)[13,14]. Understanding the relationship between structure and function is one of the main interests in the molecular biosciences. Apart from their obvious biological importance, understanding such biological processes also has the potential to unlock a number of technological innovations. For a number of biological systems it is not possible to prepare the single crystal samples needed to perform diffraction measurements. BioXAS allows both structural and electronic information to be obtained for such cases.

Other fields which are benefitting globally more and more from the proliferation of synchrotron sources are archaeology and cultural heritage science, with an rapidly growing number of synchrotron radiation-based projects[15]. X-ray diffraction and XAS allow both the identification of chemical compounds as well as the possibility to reveal mechanical or heat treatments such as firing or hammering, which can, for example, reflect the technological state of a civilization under study[16]. Such studies benefit highly from the high spatial resolution offered by synchrotron radiation light.

A beamline with the above-mentioned techniques would potentially be of invaluable service to various NRF Research Themes[17] and Centres of Excellence[18], including the following:

- NRF Research Theme 3: Geological heritage (XRD) and NRF Research Theme 7: Health (Protein crystallography and BioXAS)
- NRF Centres of excellence: Catalysis (EXAFS), Strong materials (XRD and EXAFS), Biomedical TB research (Protein crystallography and BioXAS)

It is important to stress that with the implementation of a beamtime sharing agreement with the host synchrotron, as mentioned at the beginning of this section, a host of different techniques would be available to cover other research needs.

In South Africa there is growing interest in synchrotron radiation from industry. Prominent examples which would be well served by the beamline are the investigation of catalytic processes in Fe Fischer-Tropsch catalysts by EXAFS, high resolution powder XRD to establish the structure of Fe-carbide phases in Fisher-Tropsch Catalysts (both for SASOL) and the study of fuel pellets (coating, diffusion studies etc.) for the Pebble Bed Modular Reactor (see Ref. 11). Element Six (ex - De Beers Industrial Diamonds) have also expressed interest in the possible applications of synchrotron light in materials characterisation.

## 4. Growth of the user base

A most important requirement for a successful beamline is a solid base of researchers who utilise the instrument. One of the primary tasks of a South African synchrotron initiative and this instrument will be to accelerate growth and to strengthen this user base. A large number of South African scientists are already interested in synchrotron radiation, as evidenced by the attendance at the *Science at Synchrotrons* workshop held at iThemba Labs in February this year. South Africa already possesses a small but active community of synchrotron users (26 user experiments in 2006) and interested people (78 delegates at the Feb'07 *Science at Synchrotrons* series of meetings)[11].

The importance of any initiatives that increase the number of South African scientists interested in synchrotron radiation and augment their capability to use it, must be stressed and encouraged. Examples of this would be an Annual School and Users Meeting (the first of which was the above-mentioned *Science at Synchrotrons* workshop) and the near-annual ICTP school on synchrotron radiation[19], held in Trieste, Italy, for which funding to attend for African researchers is readily available from UNESCO and the IAEA. Plans are already underway to send two students to the US Particle Accelerator School in the USA, for training in accelerator science and technology, with the course costs and accommodation being covered by the school. Similarly, other mechanisms that would allow South African users access to synchrotron facilities, would be of great benefit in this regard. One such example is the NRF-coordinated Synchrotron Development Fund under the current Knowledge Interchange and Collaboration (KIC) programme.

As mentioned in the previous section structural biology in South Africa is severely hampered by limited synchrotron access. South Africa is making rapid strides in raising its structural biology profile with the appointment of a research chair and the emergence of programmes at several universities and the CSIR. A short term solution that would significantly enhance the ease of access to synchrotrons by the rapidly growing structural biology community would be to buy a stake in an existing beamline. At present the acquisition of a portion of the ESRF beamline BM14 is under serious investigation. An annual fee of approximately ZAR 1 million would cover the costs of access by South African scientists as well as fund a South African postdoctoral researcher at the facility. This intermediate step is Stage 2 in the proposed Synchrotron Roadmap[11], and would precede the proposed South African beamline that is the subject of this study.

## 5. Location

The construction of the South African instrument in Europe, or in its vicinity, has various benefits. Apart from Europe being the easiest and cheapest location to travel to for South African scientists the negligible time difference is an important factor for projects where scientists are usually expected to work substantial hours. A beamline in Europe would also allow its staff access to other European beamlines, a fact which could also be exploited by SA users.

The newly constructed synchrotron SOLEIL in Orsay, Paris, France (first beamline open to users, September 2006) is along with the UK facility, DIAMOND, one of the latest 3rd generation synchrotron sources to open and thus provides higher brilliance than older sources. It benefits from the vast synchrotron experience of the French scientific community (it replaces the LURE source). The European Synchrotron Radiation Facility (ESRF) is also based in France. A strong collaboration already exists between the emergent South African synchrotron community and our French counterparts. They have already played a leading role in the meetings and workshops to date in South Africa, and appear keen to host our instrument.

SOLEIL is the logical choice for the above reasons. There are however a number of other sources that could be considered such as Diamond (UK), Elettra (Italy), SESAME (Jordan) and the Australian Synchrotron. This depends on the arrangements that can be made with each source as regards funding, infrastructure support and in particular for the exchange of beamtime with other beamlines.

## 6. Timescale

The outline of the various steps and the time needed for each is:

- Initial design of beamline, based on scientific needs: 6 months
- Detailed technical design of beamline: 6 months
- Beamline construction: 18 months
- Beamline commissioning: 6 months

Total = 3 years

As the beamline would be built at an established synchrotron it is possible to decrease the overall time needed. This is because experience already exists in the design of, for instance, the insertion devices best suited for XRD taking into account the parameters of their particular electron beam. It is now possible to purchase the major part of the optical components of a beamline already pre-assembled. It is clear that after the decision to build a beamline is made, it takes 3-5 years to arrive at the point where users can conduct experiments at the beamline. This strongly suggests that an early start to this project is essential. Figure 3 Timelines leading to synchrotrons being open to users at LNLS (Brazil), SESAME (Jordan) and the Australian Synchrotron.shows the progress of the synchrotron programmes in Brazil, Jordan and Australia, indicating when, for Brazil and Australia, they acquired beamlines at other synchrotron sources.

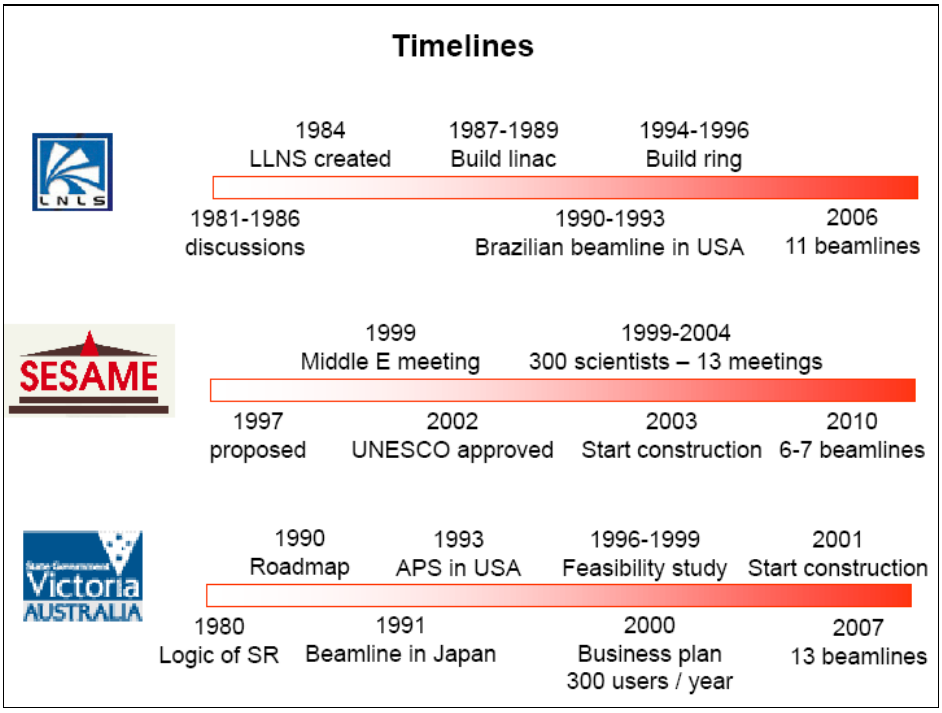


**Figure 3** Timelines leading to synchrotrons being open to users at LNLS (Brazil), SESAME (Jordan) and the Australian Synchrotron.

## 7. Staff

The beamline would require staff, both to build and maintain the instrument as well as to aid South African users in the execution of experiments. The staff would also be in the position to gain a great deal of experience in the use of synchrotron radiation. As such they will be of much benefit to collaborating South African research groups, helping in the writing of experimental proposals (see section 8) and the analysis of data. The beamline staff could possibly consist of: 2 beamline scientists and 1 or 2 postdoctoral fellows. The postdoctoral fellows will gain valuable experience in the operation of a beamline and the use of synchrotron radiation. Doctoral students from South African universities should also spend portions of each year at the instrument, conducting experiments and gaining experience, and the rest of the time at their home institutions.

It is envisaged that the beamline will continually host medium-term visitors from South African institutions, to offer in-depth experience of the use of synchrotron radiation.

It would be most beneficial to have an agreement with the host synchrotron for technical (mechanical, electronics and IT) support, primarily as a cost saving measure, but also as they would be very familiar with the particular instrumental requirements of their home facility. The option of a South African technician or engineer being based in addition at the beamline, in particular to gain experience of the relevant technologies, could also be explored.

 

## 8. Estimated cost

The costs detailed here are very rough estimates. Detailed figures can be more easily calculated when the exact beamline type, location etc. have been decided. As is discussed below many possibilities exist to gain substantial external funding from various sources to help offset these costs. With regards the initial and running costs the greatest effort must be given to finding and developing home-grown companies that are able to deliver the equipment needed. Not only will this develop the country's technological infrastructure but it will also serve as a boost to the economy. The costs (in some cases in Euros, 1 € = ZAR 10) are divided into:

- Initial: (until normal user operation, spread over approximately 3 years - see Timescale) We estimate approximately ZAR 25 million based on the average cost of other beamlines already constructed or under construction (ZAR 28 million (APS, USA)[20]; ZAR 29 million (ALBA, Barcelona)[21]; ZAR 32 million (ALBA, Barcelona)[22]; ZAR 35 million (Canadian Lightsource)[23]). A slightly reduced number has been given, based on the possibility of a portion of the initial outlay being carried by the host institution (for example the front-end, or other equipment at the interface between the synchrotron and the beamline). This initial, once-off amount is obviously the major part of the costs. If necessary this can be partially spread over a longer period, with some of the functionality of the beamline being implemented only after the first 3 years.
- Annual running costs: ZAR 600 000 to 800 000. These figures are roughly taken from the running costs of some beamlines at Elettra (Trieste, Italy). Obviously any increase in this amount would result in a better service to scientific users and increased efficiency in and quality of research.
- User expenses: If we estimate say 30 user experiments a year at 2 to 3 users per experiment, and budget ZAR 12 000 per user (the major part of that being travel) we arrive at ZAR 900 000. We emphasise that these travel costs would be the same with any other kind of synchrotron access programme, such as sharing beamtime etc.
- Staff: We assume a possible salary for someone living in France: 2 scientists @ € 3 500/month plus 1-2 postdoctoral fellows @ € 2 500/month + 30% for insurance, pension etc. = ZAR 1.48 to 1.87 million/year
- Visitors: For 2 visitors for 3 months and 2 PhD students for 3 months we arrive at ZAR 176 000. The breakdown of expenses is: return air ticket = € 800; accommodation = € 450/month; food etc. € 25/day.

An important consideration in the costs is the possibility to obtain funding from external (non-South African) sources. These could include UNESCO, various SA-country agreements, the JAPAN-outreach programmes, and possible financial help from the hosting synchrotron, in particular in the construction of the beamline and with regards to running expenses such as electricity, liquid nitrogen and the cost of user accommodation.

Based on the ongoing UNESCO support for SESAME as a regional project, the possibility of their providing funding would thus most likely be significantly increased if it was to include scientists from the greater Southern African region (or the entire continent). The IAEA could also be a source of funds, particularly for training. They are providing about US $ 1 million for the SESAME project in the Middle East, with particular emphasis on the training of the SESAME scientists[24].

The interest of industry has previously been discussed and would provide another possible source of funding. Service projects would bring in revenue and in the case of collaborative projects industry could cover expenses or purchase equipment needed for the project that would afterwards remain at the instrument. Although the cost of beamtime for proprietary research is substantial, with an eight hour shift of beamtime costing in the region of ZAR 12 500 (reference 20) to ZAR R17 000 (reference 25), which equates to a full week costing approximately ZAR 310 000, it is not high when compared with the cost of analytical services by speciality companies. The instrument would, in the case of such industrial R&D projects, in effect be generating income, while increasing the international competitiveness of South African industry.

## 9. Access for users

There would be a small number of South African based synchrotron experts, their aim being to help South African scientists interested in accessing the beamline (or any other beamlines at the same source available in the beamtime swapping arrangement detailed before). This would include help in selecting the correct technique for a particular scientific problem as well as in the drafting of a scientific proposal. As a number of international synchrotron experts have offered their help in this regard (see list of delegates in reference 11), we would also be able to take advantage of this opportunity.

Research groups wishing to conduct experiments would write such proposals detailing their proposed work. As is the general practice at international large facilities, these proposals would then be reviewed by independent (South African or international) experts taking into consideration the following criteria:

- The scientific merit of the proposed project
- The need for synchrotron radiation
- The track record of the investigating team

Additional merit could be given to projects originating from scientists new to synchrotron radiation research and those that involve students or young and emerging researchers, as a means to increase the user base and the number of people skilled in this area. Accepted proposals would then receive funding (travel and expenses) for the selected research groups to carry out the proposed work. A similar system has, for example, been an important part of the synchrotron development in Australia[7].

## Acknowledgements

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1. A brief introduction can be found at: http://www.esrf.eu/UsersAndScience/Publications/Highlights/2002/Imaging/IMA4, see also http://www.esrf.eu/UsersAndScience/Experiments/Imaging/ID17. Two similar beamlines are under construction in Canada (http://www.lightsource.ca/experimental/bmit_2.php and http://www.lightsource.ca/experimental/bmit.php) and another in Australia (http://www.synchrotron.vic.gov.au/content.asp?Document_ID=4636).
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25. Bryan Doyle, private communication (confidentially with company in question prevents further details being discussed)