Decadal Plan for Physics

X-Rays of the Future: An Australian Energy Recovering Linac

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Introduction

X-ray and neutron radiations are the salient tools to investigate matter all the way from a sub-atomic scale of the size of a nucleus through nano and micrometer extensions to macroscopic entities like engineering devices or tree dimensional whole human body mapping. A similar huge span of magnitude is valid on the time scale, where these techniques allow to track oscillations of a single electron to processes lasting hours, days or years – wherever one wants to set the limits. Correspondingly, these techniques span a wide range of disciplines ranging from nuclear physics, solid state physics, materials science, chemistry, pharmacology, geology, environmental sciences, biology, medicine, paleontology, forensic sciences, cultural heritage and engineering. Without these two kinds of radiation, being employed since 100 and 50 years ago, respectively, the wealth of our modern society would not exist. No computers, no large airplanes, no internet, no modern drugs, no extended human life. Mankind increases, demands increase while resources decrease. We are used to the quadrupling of computer capabilities every few years. We are used to higher safety standards and undisturbed health respecting each individual person. We have increasing demands in security and counter terrorism. We want to live in a community in which leisure and service overweights the work and production. And we want to create an environment which is sustainable and conservative for future generations. Such demands can only be fulfilled and sustained with engagement in scientific research at the leading edge on an international scale.

Recently, Australia has found an internationally recognized position in neutron and synchrotron related research. The OPAL neutron source is a state of the art reactor comprising the basic park of neutron scattering instruments for the Australian and, to some extend the international user community. The Australian Synchrotron is the first attempt of such source inside the country opening up the tools for a wider community. It is a third generation, medium energy source and delivers a minimal park of instrumentation to play a role in this community. While this latter source still bears great potential to be expanded, it does not play a world leading role in its field. Excellent beamline projects have been proposed for the Australian Synchrotron and are urged to be constructed to satisfy the immediate and medium term needs and the application to the broad community of research in the country. Many excellent researchers are still struggling with X-ray tubes due to lack of access here and overseas while a broadening into the applying community is more than overdue. However, thoughts must be undertaken, scientific studies and excellence projects supported to work towards what comes next – beyond the Australian Synchrotron.

Fourth generation sources in the X-ray regime are either the upcoming Free Electron Lasers (FEL) or Energy Recovery Linacs (ERL) in leading countries around the world. Distinguished features common for both concepts are their increased brilliance, their lateral beam coherence and the high time resolution they bear. The performance of those quantities increase by orders of magnitude, typically a factor of thousand. While free electron lasers are limited in very specialized applications, energy recovery linacs cover both a wide spectrum of advanced needs of the synchrotron radiation community and research ranging into the field covered by the former. Further, cost considerations of a well equipped ERL lies in the $ 500 Million while a FEL would cut into the $ 1-2 Billion, maybe more.

Synchrotron Radiation

Synchrotron radiation is emitted when highly relativistic charged particles, in general electrons, are radially accelerated, emitting dipole radiation. Due to the relativistic energy of that particle the radiation is directed into forward direction. In simple words, the radiation emits into the forward direction when the trajectory of the particle is bent. Such bending occurs in a bending magnet situated at one of the corners of a synchrotron storage ring. Insertion devices can be installed into the straight sections of a dedicated 3rd generation storage ring, such as a wiggler, in which alternate magnetic fields along the trajectory bend the particle beam forth and back, the intensity of the resulting X-ray beam being multiplied by the number of wiggler poles. If the wiggle amplitude is small, the particle beam spatially overlaps with the lateral coherence length of the emitted X-rays, leading to coherent superposition in the energy spectrum – the concept of an undulator, for which the intensity scales with the square of the number of poles. Third, when the undulator is extremely long and the emitted radiation high in intensity, its strong electromagnetic field can interact with the electron beam, eventually micro-bunching the electrons on a micrometer scale – which is the wavelength of X-ray light relativistically transformed into the electron system. Thus electrons travel on in well-defined phase relationships with the electromagnetic light field, causing Light Amplification by Stimulated Emission of Radiation (Laser). This is the concept of a Free-Electron Laser (FEL) in which the light intensity increases exponentially with the number of undulator poles, until saturation. While bending magnet, wiggler and undulator sources are readily available in third generation synchrotrons, X-ray free-electron-lasers (X-FEL) are just to become technically feasible in prototypes [LCLS-2011, DESY-2011].

Quality and Limitations of Synchrotron Radiation

The ultimate quality of X-ray radiation would be a single mode free-electron laser, analogous to laser radiation in the visual light regime. Research, technology and development are still far away from this ultimate goal – however X-FEL are seeing their infancy these days operating in a self-amplified stimulated emission (SASE) regime. X-ray flashes of the ultimate source would last one femtosecond. SASE flashes show this substructure in a 100 femtosecond pulse length, however far from being ultimate. Within these flashes, X-rays of a FEL are 100 % coherent and, as for any laser, occupancy per photon state is much larger than one.

Synchrotron radiation from a conventional storage ring delivers time pulses of 100 picoseconds, in special modes ultimately half of that. The lateral coherence of the radiation is inversely proportional to the angular source size and can reach values as high as 1 %. Limitations are given by handling long distances for a given spatial extension of the source and the then growing foot prints onto the X-ray optics. The limitations are directly linked to the brilliance of the source – basically the number of photons per source size and angular divergence of the beam, in a given energy interval. It is correlated inversely to the emittance of the electron beam – product between electron beam cross section and its divergence.

Therefore, highly coherent X-ray beams need smaller emittance and higher time resolution shorter electron bunches.

Limitations of the emittance in a storage ring is dominated by thermalization of the electron beam. Short and low-emittance electron bunches can be created by a state-of-the-art laser driven electron gun, which are then accelerated and fed into the storage ring. Because freshly injected electron bunches have to be merged with the rotating bunches, they are fed into a phase space element close to each other, but not exactly – which would be impossible by Liouville's conservation of phase space theorem. This is in cost of emittance, which is slowly improved again – over many turns – by lateral damping. So-called synchrotron oscillations of individual electrons average over milliseconds – many thousand turns in the ring – limiting the low emittance of a storage ring particle beam. Regarding the time regime, electron bunches spread from each other in the longitudinal direction, until they hit the border of the accelerating gradient in the synchronously rotating radio frequency field which restores them their lost energy on each turn. These accelerating pouches – according to the field gradient, the number of repulsive electrons in the bunch and other parameters – are 3 cm long, resulting in a time length of 100 ps upon traveling close to the speed of light.

Emittance and time structure of a highly optimized electron source deteriorate over time and reach equilibrium values essentially imposed by the physics of the storage ring, thus limit the beam quality of the synchrotron. In a conventional storage ring, the beam is pan-cake shaped where the horizontal size is typically one order of magnitude larger than the vertical, 100 μm and 10 μm, respectively. These limitations can be overcome in an energy recovery linac.

Advantages of an Energy Recovery Linac.

The technical and scientific aspects of an ERL have been recently reviewed by Donald H. Bilderback et. al. [Biderback-2010a, Biderback-2010b] stating all the advantages which apply to the present study. Further and consistent arguments are given by Hiroshi Kawata with regards to the Japanese X-ERL project [Kawata-2009]. Scientific and technical aspects of a German ERL project were led by Andreas Magerl in 2002 and resume the basis for development in this field [Steffens-2002; Bernhard-2002].

The source size of an ERL can be as small as 1 μm in both horizontal and vertical dimension. Not only, this is 2, respectively 1 order of magnitude smaller than in a storage ring, but the beam shape is round and symmetric. The small source size leads to highly coherent photon beams in both lateral dimensions, reaching 100 times the coherency than in today's state-of-the-art storage rings ESRF, SPRING-8 and APS [Biderback-2010a]. In terms of brilliance, these numbers scale with the same factor 100 times higher.

Lateral beam coherence can be as high as 35% which allows to perform X-ray experiments at their optical diffraction limit. This allows to focus a whole beam down to 1 nm^2, opening any unprecedented research and technology in a broadest field of X-ray applications throughout the area of nano-research. Diffraction of a single molecule, an atomic cluster, spectroscopy from a single atomistic point defect or examination of a selected apparatus in a living cell become feasible.

Time resolution can reach 100 fs and may be further, allowing for real time investigations into the 10 THz range and above. It allows to study coherent phonons, both acoustical and optical as well as any other collective solid state excitation in this range.

An ERL and FEL have comparable time averaged brilliances, however, the repetition rates of bunches, and thus the brilliance per bunch differs by 6 orders of magnitude. Meaning, the ERL is much gentler to samples where radiation deposit is a problem. Simulations predict that molecules blow apart into a plasma [Neutze-2000] being hit by a FEL pulse. In contrast, repetitive exposure over many microseconds or milliseconds form an ERL gives the specimen time to disperse heat and suffer less on radiation damage.

ERL bunches make only one single to a few turns through the ring structure. Then the kinetic energy is extracted and the bunch is disposed and renewed. This concept allows to perform particular treatment of the bunches which, in a storage ring, would deteriorate their performance on subsequent turns. High quality bunches shall be used at the beginning of the circuit, while further downstream bunches can be treated in an extreme way only influencing beamlines even further downstream. The upstream beamlines would be unaffected of this. For example, trajectories could be varied over a large angle in order to scan the resulting X-ray beam in the nanosecond regime.

The round geometry of the electron beam is particularly beneficial to implement helical undulators to obtain circular polarized X-ray beams, critical i.e. for magnetic scattering in all its variants.

Principles of an Energy Recovery Linac.

This concept of one turn trough a storage ring lattice is the scope of an ERL. While continuously accelerating a 100 mA beam of electrons to an energy of 5 GeV and subsequent dumping, requiring mains power of 500 MW, inefficient and costly, impractical in operation, the concept is to recuperate at least 99 % of the bunch energy and use it again for acceleration of the next. Technically, this is done by accelerating the bunches in a powerful linac, running them into a closed loop lattice – conceptional similar as in a storage ring – and decelerating them fed into the back end of the same linac. One component of the radio frequency electromagnetic field travels with the electrons, which gain energy when surfing on the accelerating field gradient. Accordingly, they enter the back end of the accelerator in a π-phase shift to on the decelerating of the radio frequency field, feeding their kinetic energy back into the field. This stored energy can be used to accelerate a subsequent bunch.

The quality characteristics of an electron bunch can be maintained for a few microseconds, corresponding to one turn in a storage ring – the concept of an Energy Recuperation Linac.

ERL or FEL?

While the past defines clearly the concepts of first, second and third generation synchrotron radiation, there is tendency that the upcoming fourth generation splits into sources based on a free electron laser, FEL, or an energy recovery linac, ERL. Of course, both have common aspects, like a low emittant electron source, superconducting accelerators, undulators, however, the scale and the layout are eminently different. First of all, all physical dimensions in a FEL are typically one order of magnitude longer than in an ERL; so the accelerator, the undulators, the beamlines. While the ERL builds on a ring concept with beamlines lined up successively, FEL stations are fanned out into parallel beamlines, the accelerator feeding those stations alternatively.

While the average power in the X-ray beam may be similar for both concepts, repetition rates are million times lower in a FEL than in an ERL. Correspondingly, the number of photons in a single bunch scales inversely by the same factor. This factor, which sounds excellent in the first place, will encounter enormous problems – just because of the power density deposited in a few femtoseconds. As in the visual light, such laser irradiation will interact strongly and non-linearily with matter. Thus, ablation occurs, plasmas are created, electrons are ripped off their atoms and follow the electromagnetic filed of the light wave. No-one can really predict, how X-FEL radiation interacts with matter and how the X-FEL optics shall be realized withstanding severe radiation damage. Similar problems occur on the detector side, how to handle such flux of information. X-FEL radiation certainly will open fundamentally new possibilities and concepts exist that a diffraction pattern off a molecule will be taken before the atoms plasmarize, it may be too far away from deeper applications in condensed matter sciences. These enormous problems to encountered will have to be solved in the first few decades of X-FEL radiation. In contrast, ERL radiation will offer enhanced possibilities to the fields of research we are performing nowadays at third generation synchrotron sources. It covers the whole range, from conventional X-ray characterization with new parameters, as time, resolution, speed, multi-dimensionality with an un-precedented accuracy to push those applications and the knowledge learned to the forefront in its field.

It is interesting to observe the fact, that the FEL concept has been developed before the ERL. The first X-FEL see their childhood in these days while the ERL realizations still lack behind. More interesting to note, that those nations having developed the X-FEL, USA, Japan and Germany, are pushing and leading X-ERL development. The scientific community of those countries has realized the orthogonality of both concepts and is reacting to this.

In Australia, research priorities are very applied, not to develop novel facilities, but to solve problems. An ERL can be used in the widest sense of X-ray analysis and across the disciplines. Therefore, the next natural instrumental development, but essential step beyond the Australian Synchrotron is to build an Energy Recovery Linac.

Applications

Quantum Nanoscience

A completely new application of ERL radiation would be in the field of quantum computing, quantum metrology and quantum nanoscience [Milburn-2008]. In the past, it has been demonstrated that response from coherent ultrasonic waves in crystals can be resolved in time and space by high resolution synchrotron radiation techniques. At low acoustic frequencies 0-100 MHz), strain fields are seen [Liss-1998], while coherent phonon states separate into satellite peaks in the gigahertz range (0.1-10 GHz) [Liss-2003]. Subsequently, lattice cell changes of optical phonons have been measured in real time of terahertz stimulation, demonstrating the oscillations of atoms on neighboring lattice sites against each other – that what distinguishes an optical phonon [Sokolowski-Tinten-2003]. Last not least, X-ray photons have been successfully stored in crystal cavities [Liss-2000] which were recently miniaturized into Fabry-Pérot interferometric devices [Chang-2007]. Nowadays, it is possible to design and built devices on the nanometer scale, on which quantum mechanical properties play an ever increasing role.

The correlation lengths of a quantum state, whatever it is, range into the same order of magnitude, the nanometer scale, why quantum effects will be potentially employed in future applications, such as quantum computing. Novel X-rays, as produced from an ERL, focused down to the nanometer, highly coherent, then will allow to probe matter within one given quantum state. Quantum experiments would be performed as conventional, while they are additionally probed locally and at a given moment in time by X-rays. Kippenberg and Vahala [Kippenberg-2008], for example, describe opto-mechanical devices, in which photons in a resonator strongly couple to mechanical oscillations of a nanometer sized mass-spring system. Such monolithic devices will be probed by ERL X-rays, which routinely detect atomic displacements on the femtometer scale. Last not least, an X-ray photon is a wave and will contribute to the quantum mechanical system, which may be used to tailor impose a quantum structure to the X-ray beam for probing another in an echo effect. Further, high intensity, coherence and time resolution of an ERL beam may be used to probe quantum states as they are today well established in our labs. For example, a single Cooper-pair passing in a superconductor will be imaged revealing novel experimental evidence for the understanding of superconductivity. Similarly, no-one has a clear understanding of how atoms are arranged in a Bose-Einstein condensate. Again, ERL X-rays will probe. One can argue, that the diffraction of X-rays may disturb such systems, however, including the X-ray photon into the quantum mechanical model of the whole system will give unique and unprecedented information about the whole. The whole spectrum of X-ray methodologies, including diffraction, imaging, fluorescence, nuclear resonant scattering, dichroism, spectroscopy will be available and the application of such characterization technology into more complex coherent quantum systems is just a question of time.

Amorphous materials

Despite their abundance and expanded long term research, the understanding of glasses and amorphous materials is still very controversial. Early predictions like the local icosahedral symmetry in simple metallic liquids and glasses became experimentally accessible only in the past decade by usage of highly advanced synchrotron radiation [Reichert-2000]. Correlations between the mechanical shear strength and the glass transition have been universally established empirically, however, an atomistic approach was found experimentally only very recently [Qu-2011]. The authors demonstrated upon thermal expansion that second nearest neighbors relatively expand faster than first nearest neighbors, which involves shear in the building blocks and essentially corresponds to a stretching of zigzag chains. Most evidently, the isotropic orientation of the locally anisotropic building blocks leads to local stresses which yield at the glass transition, leading to all the well known effects like the increase of free volume, decrease of stiffness etc. Experimentally, the atomic strain of the atomic shear and the yield strain of a macroscopic compression test have been found to be equal, proving this atomistic behavior.

Hundreds of questions established by theoreticians to be addressed experimentally follow, demanding high quality, hard X-ray radiation. What are the species of nearest neighbors, what is the energy landscape, the dynamics and kinetics. Are the metallic glasses homogeneous or coexisting of different phases, nanometer scaled. How is the situation in ionic liquids and glasses as relevant for our minerals industry, energy storage materials and so on. Are the same concepts valid for polymers? These very fundamental questions will profit enormously from superior beam qualities of nanometer size, coherence, time resolution, intensity. Shear banding is often a localized, catastrophic phenomenon. Depending on the material and situation, controlled flow can happen – or catastrophic melting of the zone with temperatures reaching 10^4 K. Anything is possible and absolutely no in-situ experimental data on these nanometer extended bands forming on nanosecond time scales exist to support any model.

Nanometer sized beams will be used to probe local structures such as in above mentioned zones. Time resolution will give unprecedented data about temperatures, flow, atomic rearrangement during the flow happening. Emerging techniques using coherent diffraction, such as X-ray speckle pattern are evaluated by a cross correlation analysis to uncover local symmetries in disordered matter [Wochner-2009].

Hard and High Energy X-Rays

Conventional storage rings are often designed to compromise the hard and high-energy X-ray regime in favor for enhanced beam properties in the lower energy X-ray regime. Applications are yet dominated by the soft matter communities. However, high energy X-rays have tremendous advantages in materials research and materials physics [Liss-2003] and state of the art developments all go towards higher energies. The main argument for higher energies is the smaller absorption and the higher penetration into heavier materials. However, the trend to high-energy X-rays is even the case for applications of the classical low energy beamlines, where absorption would not play a role. Here the other advantages hold, as a small curvature of the Ewald sphere, large reciprocal space coverage, forward scattering, large focal and detector distances for complicated sample environment. Thus surfaces, interfaces have been studied in realistic environments, such as the oxidation of nanoparticles [Nolte-2008]. Radiation damage is low on soft matter, protein crystals and deep reciprocal space coverage allows for very fast scanning methods. The latter holds in general where full three-dimensional reciprocal space mapping is necessary, which becomes intrinsically fast on undulator beamlines, as feasible at an ERL, because only one axis needs to be rotated. Full reciprocal space data leads to inherent novel information in many fields of application, a method which is just in its childhood. Applications lie in the investigation of diffuse scattering of any distorted material [Welberry-2010], texture measurements in engineering processes, crystallography, reflectometry on thin layers, to mention but a few. Engineering applications such as physical thermo mechanic simulations are developed nowadays using a synchrotron beam [Liss-2010], however, time structures of intense sources will offer measurements like shock impacts on the nanosecond scale – applications from earth quake simulation to laser surface peening. Already nowadays, the fastest X-ray tomographies are performed with high energy X-radiation. ERL beams will allow for enhanced sources, undulator radiation, circular polarization, brilliance, flux at the sample to enable unprecedented time resolved studies in realistic environments. In-situ and in real time!

Time resolved scattering

High brilliance ERL pulses of X-rays will allow to probe for time resolved measurements covering from the femtosecond timescale to many hours or days. Depending on the scientific question and phase space / time coverage, time scales of anything below a millisecond are most challenging for existing technologies. Thus, a < 100 fs pulse is needed to stroboscopically record gigahertz to terahertz excitations in a solid [DeCamp-2001, Reis-2007]. Such stroboscopic data acquisition has been used in many situations, however, the shortness of the bunches gives access to unprecedented time resolution. Further, X-ray flashes from bunch trains highly charged with electrons will continuously probe on the nanosecond time scale for non-repetitive examinations. Bunches loaded with photons will repeat every 2 ns in order to record a pump-probe experiment, such as a shock impact or a laser excitation in a bulk of material. Gigahertz two-dimensional high-speed cameras are already available for the optical light and will be there for X-rays well before the timescale of construction of an ERL. Alternative detection methods are streak cameras or moving source concepts. In the latter, the electron trajectory of the ERL ring can be modified from bunch to bunch, such that dispersion at the sample can be used to achieve recordings of these high frame rates. Last not least, it will be necessary to scan thee dimensions of real or reciprocal space for tomography or total diffraction experiments. Full rotations of samples shall be done on the microsecond time scale while probing highly angular resolved frames in nanoseconds.

Applications range through the whole field of X-ray technology wherever time resolution is needed. It can be equally employed to spectroscopy, diffraction, speckle correlation, imaging – or even their combination. Scientific questions may be heat transport through thin layers, melting mechanisms, study of diffusion, multiferroic switching and interaction, order / disorder transitions, phased transformations, martensitic transformations, quantum systems, coherent phonon switching, biologic cell apparati, nuclear spin correlations and much more.

As an example, X-Ray diffuse scattering with a femtosecond resolution has been applied to the study of nucleation dynamics from the liquid in a laser ablation process [Lindenberg-2008]. Phonons in the multiple gigahertz range have been recorded by X-rays in real time to understand the bond softening in bismuth [Fritz-2007] to open access into the field of phonon engineering. Here, the group around Kazutaka Nakamura use femtosecond laser pulses to start and stop coherent phonons in crystals and make them switchable [Takahashi-2009].

Coherent imaging and diffraction

The high lateral coherence of an ERL X-ray beam will be a milestone for the activities in the field of coherent imaging. Australia has already world leading expertize and runs a competitive research program, the ARC Centre of Excellence in Coherent X-ray Science, headed by Keith Nugent [CXS-2011]. The program ranges from fundamental problems in X-ray optics, through enhanced structural determinations to applications in biological and medical sciences. Detailed enumeration would explode the frame of the present manuscript and the reader is referred to this project, which largely depends on access to fourth generation facilities.

Earth – Wind – Fire – Water

The seemingly infinite breath in the application of X-rays makes this proposal a necessity throughout the fields of earth based experimental physics, delivering unprecedented inputs into the even broader community. In particular, ERL radiation will serve all four Clusters established for this Decadal Plan: ***Earth:*** Condensed matter and materials physics; Energy and power technologies; Chemical physics benefit already nowadays strongly from synchrotron X-ray diffraction techniques to which novel ERL radiation will contribute tremendously towards a comprehensive understanding of the details, necessary for the goals of these disciplines. ***Wind:*** The enhanced X-ray source bears potential for direct applications in spectroscopy related to atomic physics, plasma physics and nuclear physics. ERL radiation will be brilliant enough to study single atoms, correlations in plasmas nuclear excitations. The existing activities in those fields will be directly projected to the shorter time scales, the radiation density and the coherence. ***Fire:*** As presented in an example, absolutely novel approaches are opened by an ERL to the fields of optics and photonics; quantum information; quantum computation to which phononics adds. In the same way as under the Earth cluster, such kind of radiation will be used for an enhanced understanding in biophysics, where probably a major filed of application is settled. ***Water:*** Australia has already leading knowledge employing synchrotron radiation for phase contrast imaging of light tissues, which will be strongly enhanced by an ERL. Climate and atmospheric physics will be supported by X-ray based characterization techniques. The ERL beam quality is inherent for high pressure experiments of the geophysical community. Acoustic waves and shock waves have been probed and visualized by X-rays, while an ERL will contribute to study such phenomena systematically, related to hypersonics, fluid mechanics, and geophysics. The whole spectrum of application will be available to industrial users and industrial physics.

Conclusion and Recommendation

A fourth generation X-ray light source is necessary to establish and sustain competitive advantage of the Australian Physics Community at the forefront of international science. An Energy Recovery Linac (ERL) will deliver unprecedented time, spatial and reciprocal space resolution and coverage. Investigations span though all the four clusters, Earth, Wind, Fire and Water, established for the Decadal Plan 2011.

Action must be taken immediately to establish a working group and a comprehensive scientific case and to participate in the international community, such as in dedicated design workshops. A scientific and technical design report shall be established within one year in order to possess a running and producing facility well before the end of the decade. The concept shall be propagated in the Australian research community through national meetings, university teaching, presentations to the public, including schools and industry.

Long term benefits of such large research infrastructure are not only new discoveries at the forefront of science, but also technological developments which will settle in Australia. Other countries with a history of similar large facilities, advanced in their time, have seen a boom of local technology, such as superconducting devices, detectors, optics, mechanics, high precision technology to mention but a few.

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