Executive summary

1 Basic objectives

This report contains a full technical description of the European X-Ray Free-Electron Laser (XFEL) Facility, a new international scientific infrastructure to be built in the north west of Hamburg. The purpose of the facility is to generate *extremely brilliant* (peak brilliance ~ 10^{33} photons/s/mm^2/mrad^2/0.1%BW), *ultra-short* (~ 100 fs) pulses of *spatially coherent* x-rays with wavelengths down to 0.1 nm, and to exploit them for revolutionary scientific experiments in a variety of disciplines spanning physics, chemistry, materials science and biology. The design contains a baseline facility and provisions to facilitate future extensions and improvements, in preparation for further progress in the relevant technologies. The basic process adopted to generate the x-ray pulses is Self-Amplified Spontaneous Emission (SASE), whereby electron bunches are generated in a high-brightness gun, brought to high energy (up to 20 GeV) through a superconducting linear accelerator (linac), and conveyed to long (up to ~200 m) undulators where the x-rays are generated. Five photon beamlines deliver the x-ray pulses to ten experimental stations, where state-of-the-art equipment is available for the experiments.

From this new user facility, novel results of fundamental importance can be expected in materials physics, plasma physics, planet science and astrophysics, chemistry, structural biology and biochemistry, with significant possible impact on technologies such as nuclear fusion, catalysis, combustion (and their environmental aspects), as well as on biomedical and pharmaceutical technologies. Thanks to its superconducting accelerator technology, in spite of competing American and Japanese projects, the European XFEL Facility will allow Europe to keep its leadership in basic and applied science with accelerator-based light sources, a leadership it acquired in the early 90s with the construction and operation of the European Synchrotron Radiation Facility (ESRF) in Grenoble.

2 History of the project

The basic technology underlying the European XFEL Facility is the superconducting linac technology, developed by an international collaboration coordinated by the Deutsches Elektronen-Synchrotron (DESY) laboratory in Hamburg, with the initial objective to create a Tera-Electronvolt Superconducting Linear Accelerator (TESLA), an electron-positron linear collider with TeV energy, for particle physics studies, hence, the name TESLA technology. It was soon realised that this type of innovative linac had ideal characteristics for an x-ray free-electron laser. Proposals to build a free-electron laser, first as a side branch of the linear collider, and later as a self-standing facility, were put forward by DESY to the German government. The construction of a test facility (TESLA Test Facility 1, or TTF1) was undertaken, and lasing down to ~90 nm wavelengths was successfully demonstrated in 2000. TESLA Test Facility 2 (TTF2) had the more ambitious goal to push lasing to 6 nm wavelengths, with a 1 GeV linac. This should be achieved in 2007; in the meantime, acceleration of electrons up to 0.75 GeV resulted in lasing at 32 nm (January 2005) and at 13 nm (April 2006), and a vigorous user programme was started in August 2005 in the experiments hall downstream from the free-electron laser, forming what is now called the Free-electron LASer in Hamburg (FLASH) facility. In 2003, the German government decided to launch the proposal to constitute a European facility for the construction and operation of an x-ray free-electron laser in Hamburg, undertaking the commitment to finance the new facility by providing up to 60% of its construction costs, and up to 40% of the operation costs. The choice of the location in Hamburg is motivated by the possibility of taking advantage of the unique experience and know-how of the DESY Machine Division in the area of superconducting linacs, and of the possibility of gaining first-hand experience on the operation of a free-electron laser (FEL) through the FLASH facility.

3 The scientific case and the X-ray FEL international context

All natural sciences benefit from the use of photons (light waves) of different wavelengths to probe the phenomena of nature. The use of infrared, visible and near ultraviolet light has been revolutionised by the invention of gas lasers and of solid-state lasers, with their properties of high brilliance, spatial coherence and, in more recent decades, ultrashort pulses, with duration down to a few femtoseconds or less (1 femtosecond, or 1 fs, equals a billionth of a millionth of a second; light travels a distance of 0.3 µm in 1 fs). This timescale is of particular importance because atoms in molecules and solids oscillate around their equilibrium positions with typical periods of a few hundreds of femtoseconds, and in general, movements of atoms during the rearrangement of their positions in chemical reactions, or phase transformations also occur on such a timescale.

In the range of the ultraviolet, soft x-ray and hard x-ray wavelengths, great progress was achieved by the exploitation of synchrotron radiation, the brilliant emission by electrons or positrons orbiting in a circular accelerator. Synchrotron radiation, however, is far less brilliant than a powerful laser, has a very limited degree of spatial coherence, and it comes typically in pulses of ~ 30 ps = 30,000 fs duration. The objective of the modern projects for the realisation of x-ray free-electron lasers is the extension of the scientific and technological revolution, ushered in by lasers in the visible light range, to the x-ray range, providing spatially coherent pulses of < 100 fs duration, with peak powers of many GW.

As discussed in four international workshops organised between October 2005 and March 2006 in Hamburg, Paris, Copenhagen, and near Oxford, the outstanding properties of the European XFEL beams (coherence, ultra-high brilliance and time structure) and the development of appropriate detectors and instrumentation will allow completely new experiments. A few examples are listed overleaf.

Coherence can be used for holographic and lensless imaging in materials science and biology. Spectacular possibilities open up, as detailed theoretical studies and simulations predict that, with a single very short and intense coherent x-ray pulse from the XFEL, a diffraction pattern may be recorded from a large macromolecule, a virus, or a cell, without the need for crystalline periodicity. This would eliminate a formidable bottleneck for many systems of high interest, e.g. membrane proteins, viruses and viral genomes. Measurement of the over-sampled x-ray diffraction pattern permits phase retrieval and hence, structure determination. Although individual samples would eventually be destroyed by the very intense x-ray pulse, a three-dimensional data set could be assembled, when copies of a reproducible sample are exposed to the beam one by one.

The high intensity can also be used to produce highly ionised states of atoms, generating in the laboratory, conditions and processes occurring in interstellar gases. In conjunction with the ultra-short pulse duration, it can be exploited in pump-and-probe experiments, where conventional laser pulses (pump) are used to trigger a chemical reaction or a phase transition, and the XFEL pulses (probe), each following the pump pulse with a well determined delay (from ~50 fs up to nanosecond or even µs), provide a "movie" of the atomic displacements and rearrangement of chemical bonds. In this way, catalytic mechanisms in chemical and biochemical reactions can be elucidated, fast reactions (e.g. combustion) can be subject to detailed investigation, nucleation of ordered phases at phase transitions can be imaged, and hitherto inaccessible states of matter can be brought to experimental investigation: if the pump pulse is sufficiently powerful to produce a plasma, the x-ray pulse can still penetrate the highly ionised medium (opaque to visible light) and provide information on the propagation of the shock front, on the time evolution of temperature and pressure distributions and on the equation of state.

As already emphasised, the potential relevance of scientific breakthroughs of this caliber extends beyond basic science, to technologies of essential importance for Europe. It would not be wise to leave a competitive advantage in this field to the United States, where the Linac Coherent Light Source (LCLS) project is well under way at Stanford, and to Japan, where the Spring-8 Compact SASE Source (SCSS) has already in 2006 obtained the financial green light for start-up. Although these projects started already, and are probably going to be completed earlier, the European XFEL adoption of the superconducting accelerator technology allows the production of 30,000 x-ray pulses per second (and possibly even more in the future), compared to the 120 of the LCLS and the 60 of the SCSS. In addition to this decisive technical advantage, reducing the time necessary to complete some experiments by two orders of magnitude, the useful experience acquired with FLASH could considerably benefit the rapid establishment of a successful scientific exploitation. If the European XFEL Facility keeps a schedule comparable to that of the competing projects, it can occupy the leading position in this field.

A European laboratory in Hamburg and Schleswig-Holstein, pursuing excellence in the physics and applications of hard x-ray free-electron laser radiation would be complementary to other projects in Europe emphasising the soft x-ray part of the spectrum, and benefit all of them through the development and sharing of common technologies.

4 Layout and performance goals of the facility

The main components of the facility are (see Figure 4.1) the:

- injector;
- linac;
- beam distribution system;
- undulators;
- photon beamlines;
- instruments in the Experiments Hall.

These components are disposed along an essentially linear geometry, 3.4 km long, starting on the DESY campus in the northwest part of the city of Hamburg, and ending in the neighbouring Federal State of Schleswig-Holstein, south of the city of Schenefeld, where the experimental hall is located.

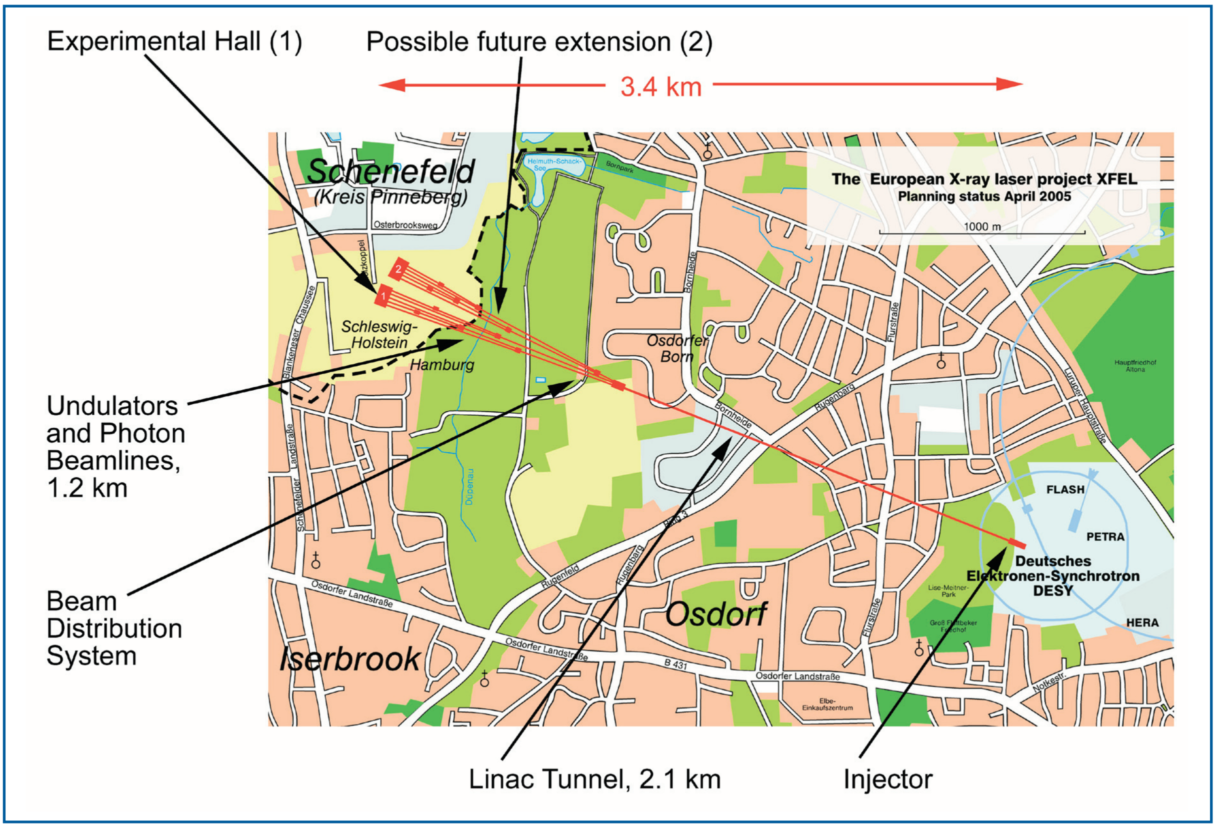

Figure 4.1 *Schematic layout of the main components of the European XFEL Facility.*

The basic functions of the main components are schematically described in the following. In the injector, electron bunches are extracted from a solid cathode by a laser beam, accelerated by an electron radio frequency (RF) gun and directed towards the linac with an exit energy of 120 MeV. In the linac, consisting of a 1.6 km long sequence of superconducting accelerating modules, magnets for beam steering and focusing, and diagnostic equipment, the electrons are accelerated to energies of up to 20 GeV (17.5 GeV is the energy foreseen for the standard mode of operation of the XFEL facility). Along the accelerator, two stages of bunch compression are located, to produce the short and very dense electron bunches required to trigger the SASE process. At the end of the linac, the individual electron bunches are channeled down one or the other of two electron beamlines by the beam distribution system (Figure 4.2). Electron bunches channeled down the electron beamline 1 pass through the undulators SASE 1 and SASE 3, producing respectively hard x-ray photons with 0.1 nm wavelength (SASE 1) and softer x-ray photons with 0.4 -1.6 nm wavelength (SASE 3), by the SASE FEL process. After going through SASE 3, electrons are deviated towards a beam dump. Electron bunches channeled through the electron beamline 2 are led through the undulator SASE 2, where hard x-ray photons with wavelengths 0.1-0.4 nm are produced by the SASE process; and then through the undulators U 1 and U 2, before ending in the second beam dump. In U 1 and U 2, very hard x-ray photons (wavelengths down to 0.014 and 0.06 nm, respectively) are generated by the spontaneous emission process. The photons generated by the five undulators are transported through the respective photon beamline to the experimental hall, where they are fed into ten experimental stations. Reducing the electron energy at the end of the accelerator would generate longer wavelengths, in case they are required by some experiments; for example, an electron energy of 10 GeV would correspond to x-rays of 4.9 nm wavelength from the SASE 3 undulator.

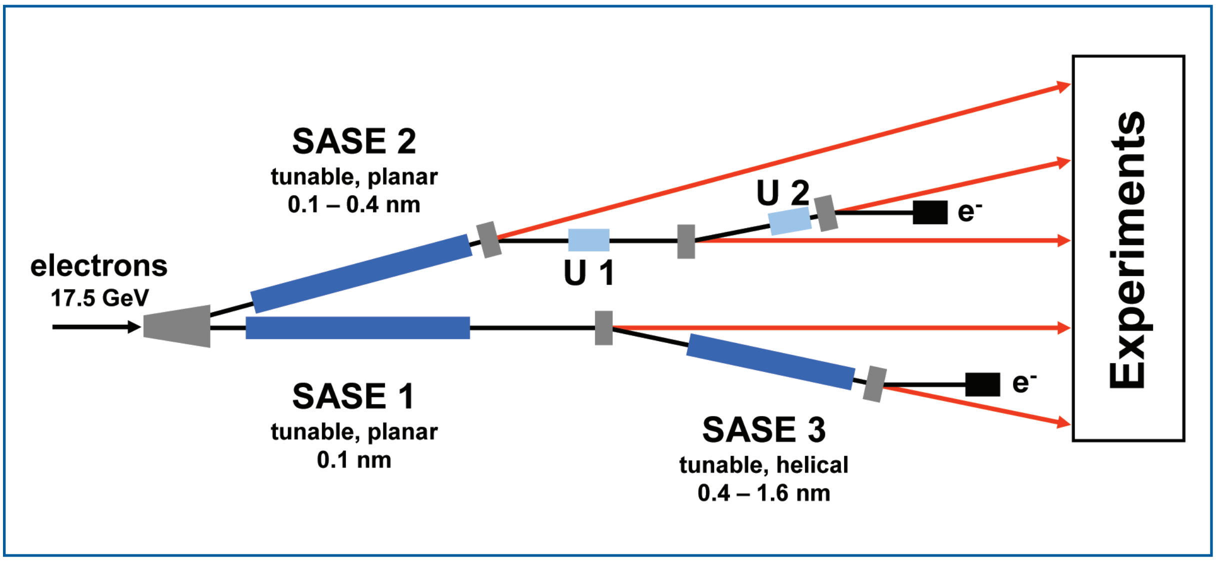

Figure 4.2 *Schematic view of the branching of electron (black) and photon (red) beamlines through the different SASE and spontaneous emission undulators. Electron beamlines terminate in the two beam dumps and photon beamlines in the experimental hall.*

The installation and commissioning of the accelerator, the undulators, beamlines and experimental stations will take place gradually, according to a strategy for the achievement of intermediate and final goals of the facility which was established with the advice of the Scientific and Technical Issues (STI) Working Group.

The first electron beamline and the SASE 1 undulator are going to be installed first. The commissioning of the accelerator and of the SASE 1 undulator, beamline and first station will be pursued, in parallel with installation of the other electron branch, until the first set of intermediate goals (see Table 4.1) is reached.

As recommended by the STI Working Group, the following criteria for the start of operation of the accelerator complex and the SASE radiators and beamlines were adopted:

- The accelerator complex and SASE 1 start operation when on SASE 1 a photon beam is obtained with the intermediate values of Table 4.1, and sufficient equipment is installed and commissioned to perform first scientific experiments.
- SASE 2 starts operation when the same criteria as above are fulfilled, for wavelengths between 0.2 and 0.4 nm.
- SASE 3 starts operation when the same criteria as above are fulfilled, for wavelengths between 2 and 6 nm.

Following the positive experience of the FLASH facility, developments towards the final project goals on all beamlines will proceed in parallel with early user operation, as soon as the criteria stated above are fulfilled.

Parameter	SASE 1 intermediate values	SASE1 final project values	Units
Wavelength	< 0.2	0.1	nm
Peak brilliance	10^{30}	5×10^{33}	Photons/s/mm²/mrad²/0.1% BW
Dimension at sample (no optics)	< 1.0	~ 0.6	mm², FWHM
Positional stability	50	10	% of beam size, rms
Photon energy stability	~ 0.1	~ 0.1	%
Shot-to-shot intensity fluctuations	Up to a factor 10	0.3 – 0.5	Dimensionless, peak-to-peak

Table 4.1 *Intermediate and final project values for the accelerator and SASE 1 undulator and corresponding photon beamline.*

5 Cost, schedule and personnel

5.1 Cost of the project

All costs from the project preparation to the commissioning phase (i.e. prior to the start of operation) have to be summed up in order to determine the total project construction cost (TPCC). There will be a period of about 2.5 years during which an overlap of construction, commissioning and operation will occur (see also the discussion of the time schedule and budget profile below). The contributions to the TPCC, summarised in Table 5.1, are:

- The project preparation costs. These are the expenses since the XFEL Memorandum of Understanding (MOU) came into effect (end of 2004), incurred by DESY and by institutes which have concluded collaboration contracts with DESY under the XFEL MoU.
- The construction costs in the proper sense, of the accelerator, the undulators, the photon beamlines, scientific instruments, civil engineering and technical infrastructure of the European XFEL Facility, including capital investment and manpower.
- The cost of commissioning the facility with beam.
- An addition to the personnel cost, in order to take into account allowances for personnel moving from their home country to work at the XFEL company.
- An additional personnel cost overhead, taking account of the XFEL company's management and support costs.

Recurrent costs during the construction in the proper sense (electricity, water, Helium) are not included in the TPCC, since they will be covered by the DESY operation budget free of charge to the XFEL project. Costs related to land acquisition are also not included in the TPCC, since Germany offered to provide the ground free of charge to the project.

Project preparation	38.8 M€
Project construction, capital investment	*736.3 M€*
Project construction, personnel	*250.1 M€*
Total construction cost	**986.4 M€**
Beam commissioning	56.4 M€
Total project construction cost	**1,081.6 M€**

Table 5.1 *Total project cost, including preparation – commissioning phases. All cost figures are on the price basis of the year 2005. - The original Table 5.1 of the TDR has been slightly re-arranged: the additional personnel cost (allowances) and the additional management overhead of the XFEL GmbH, initially shown in separate lines of the table, are now included in the cost for construction and commissioning.*

As described in detail in Chapter 10, the breakdown of this cost between the major components of the facility, is displayed in Figure 5.1.

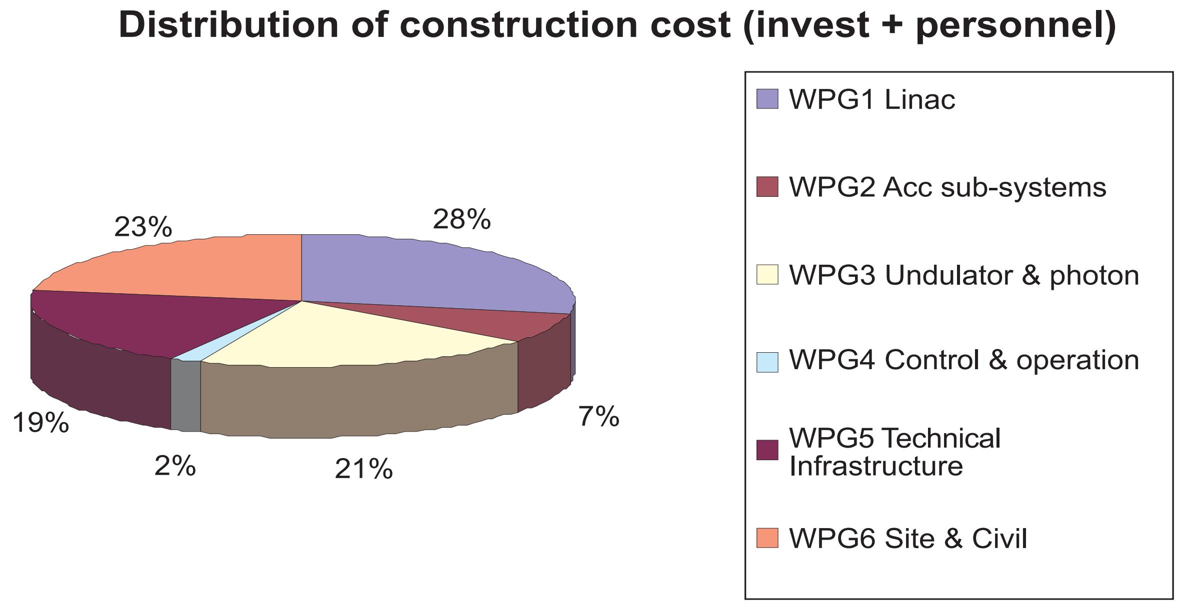

Figure 5.1 *Breakdown of the proper construction costs (sum of capital investment and personnel cost) into the work package groups corresponding to the main components of the facility.*

An analysis of the risk of overspend was performed according to guidelines specified by the Full Costing Issues (FCI) subgroup of the Administration and Financial Issues (AFI) Working Group. The resulting risk budget (8% of the proper construction costs) amounts to 78 M€, and is the additional figure required to bring the probability of successful completion of the facility within budget to 98%.

The estimated yearly operation costs of the facility, after the end of all construction, are 83.6 M€, including all recurrent costs for operation, maintenance and refurbishment, and support of the international user activities, plus a PhD student and a visiting scientists programme.

5.2 Project time schedule

The time schedule for the project is presented in Figure 5.2, which assumes that the official start of the project construction is January 2007. For each of the major parts of the facility, phases during construction (which can partially overlap in time) can be defined as:

- design, prototyping and industrialisation;
- fabrication (including pre-series);
- installation;
- commissioning (technical and with beam).

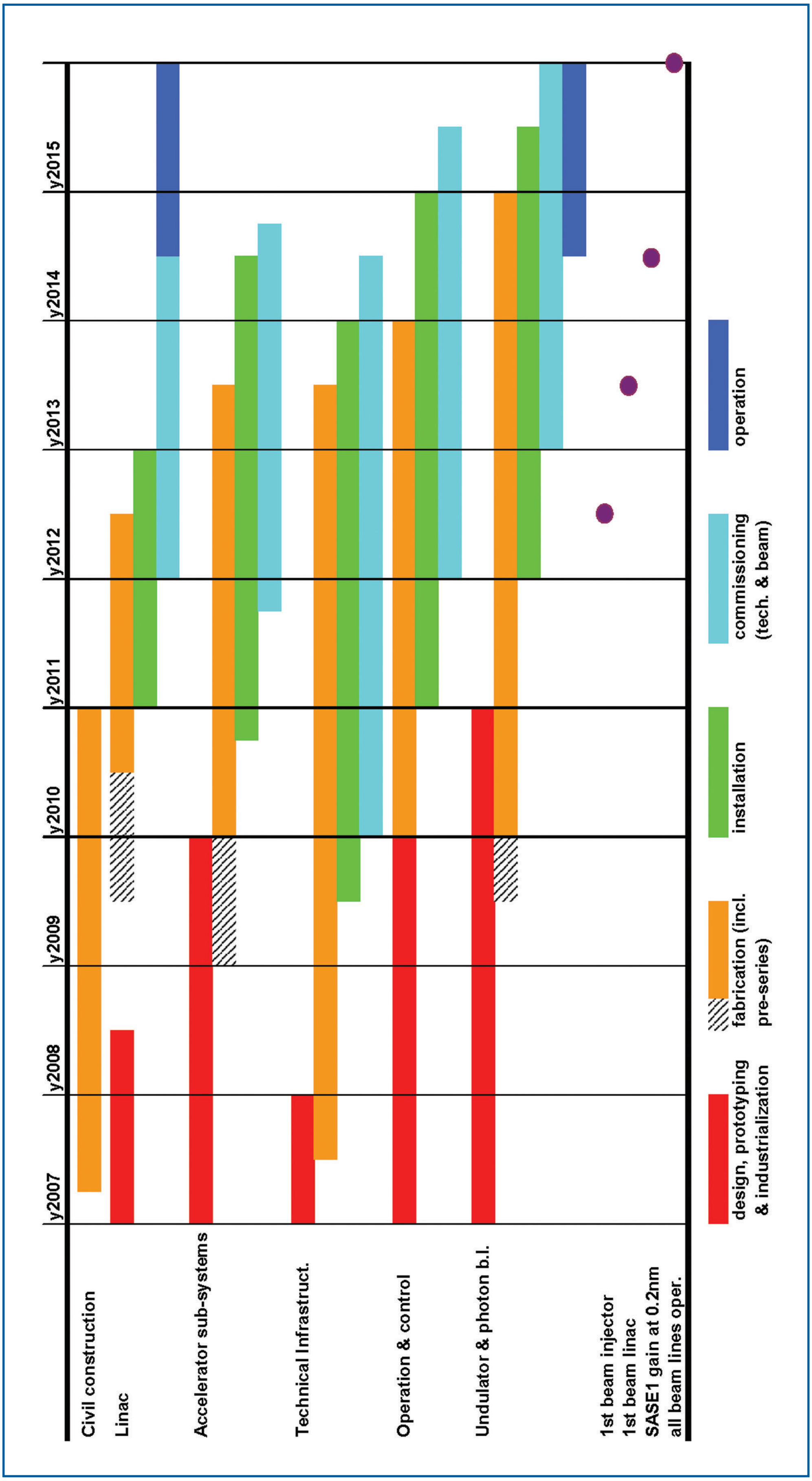

Figure 5.2 *Sketch of the schedule for the main components of the facility from start of construction to beginning of operation.*

In summary, the construction schedule provides for the milestone of first beam into the linac to be met 6.5 years after the start of construction. At this point in time, the first branch of beamlines with the SASE 1 undulator will also have been installed. Beam commissioning will then progress until the intermediate performance milestones of SASE 1 radiation are reached, 7.5 years after the start of construction. This beamline will then become operational for first experiments. Commissioning of the other beamlines follows.

5.3 Budget profile

With the different contributions to the TPCC as summarised already, the construction time schedule and the operation costs as described in Chapter 8, a complete budget profile for all phases from preparation to operation can be constructed. The result is displayed in Figure 5.3 showing the yearly budget from 2005-2016 on the price basis of the year 2005 (i.e. without applying an escalation to take inflation into account).

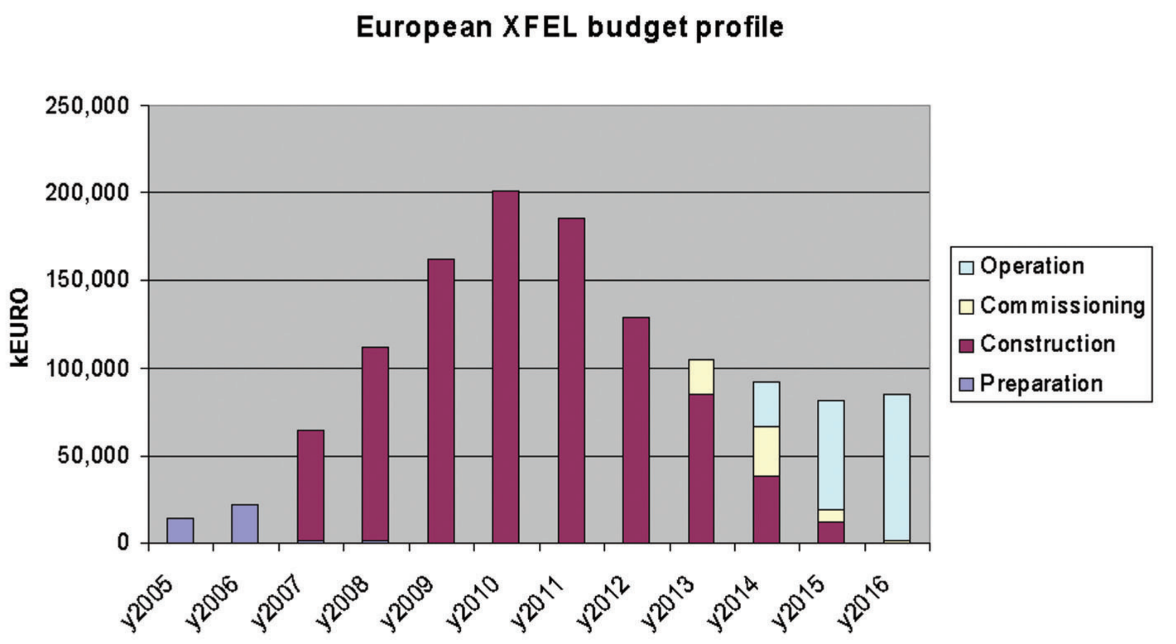

Figure 5.3 *Budget profile (sum of capital investment and personnel cost on year 2005 price basis) from preparation to operation phase of the project.*

Personnel costs, as given explicitly in Table 5.1 and implicitly in Figure 5.3 correspond to the cost of the personnel hired by the facility, plus the personnel costs for those work packages of the project, which are provided, as an in-kind contribution, by participating countries' laboratories.