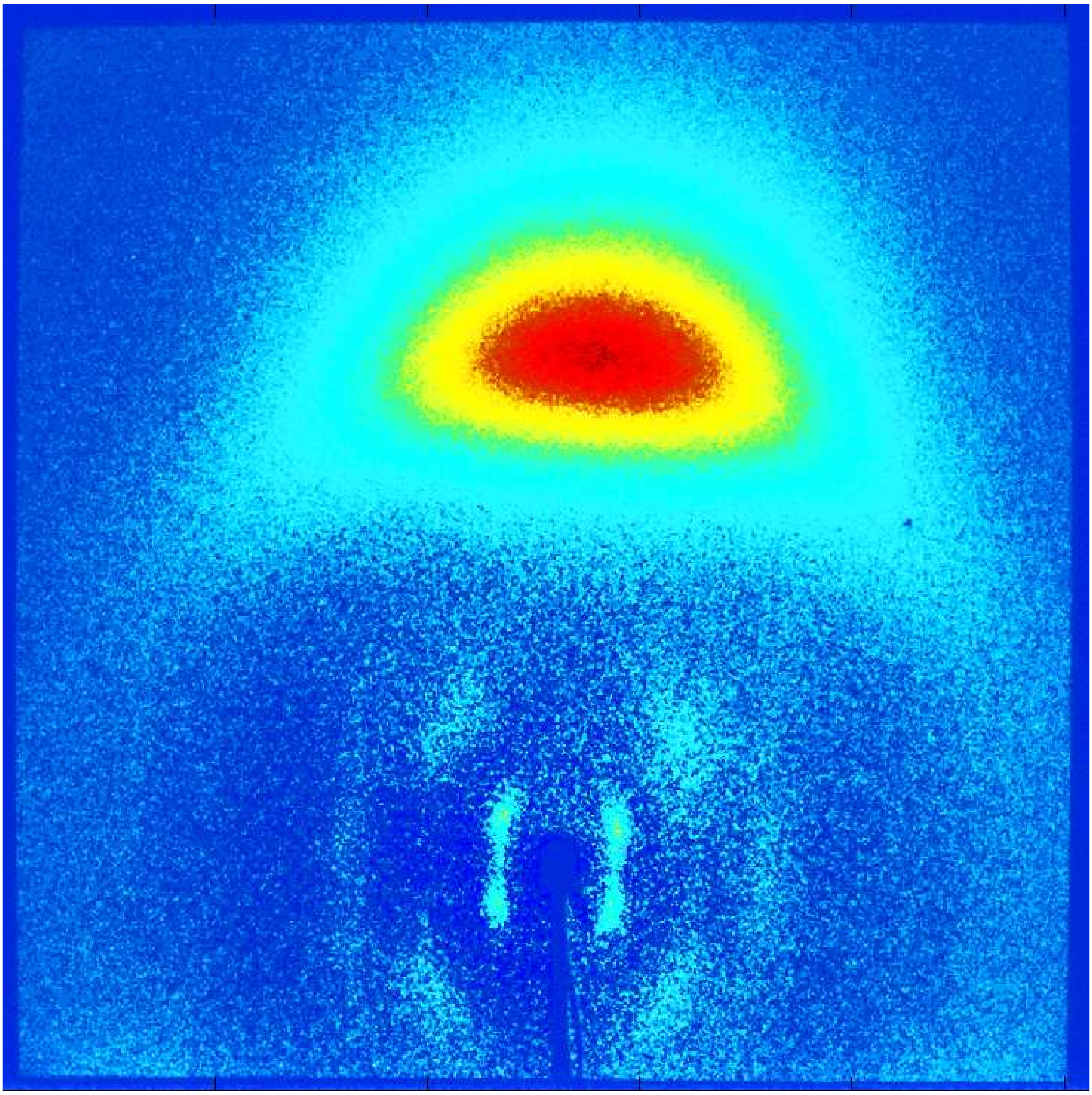
Report on the DUBBLE beamlines at the ESRF



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Acronyms

ALS	Advanced Light Source (Lawrence Berkeley Lab)
APS	Advanced Photon Source (Argonne National Lab)
BAG	Beam time Allocation Group (mechanism for rapid access to ESRF MX beamlines)
BENESYNC	Belgian Dutch consortium participating for 6% in the ESRF
CAT	Collaborative Access Team (CRG equivalent at the APS)
CRL	Compound Reflective Lenses
CRG	Collaborative Research Group
DPI	Dutch Polymer Institute
DUBBLE	Dutch-Belgian Beamlines at the ESRF
ESRF	European Synchrotron Radiation Facility
ESUO	European Synchrotron User Organization
FEL	Free Electron Laser
HRPD	High Resolution Powder Diffraction
ID	Interface Diffraction
MX/PX	Macromolecular Crystallography/Protein Crystallography
PX/MX	
SAXS/WAXS	Small and Wide Angle X-ray Scattering
SR	Synchrotron Radiation
XAFS	X-ray Absorption Spectroscopy (also XAS, XANES, EXAFS)

Summary

- The DUBBLE project consists of two synchrotron radiation beamlines at the European Synchrotron Radiation Facility that provide additional access to experimental techniques for which the ESRF public beamlines cannot provide sufficient beamtime to satisfy the requirements of the Dutch and Flemish user community.

- The DUBBLE project is co-funded by the Nederlandse Organisatie voor Wetenschappelijk Onderzoek and Fonds Wetenschappelijk Onderzoek Vlaanderen.

- The DUBBLE beamlines have in the last 10 years produced around 600 publications and PhD thesis of a high qualitative level. The annual output can be expected to stabilize around 70-80 publications/year. The beamlines are responsible for around 50% of the total Dutch and Belgian materials science publications using synchrotron radiation based results.

- The instrumentation has been upgraded in the last 3 years and it can be foreseen that the technical state of the beamlines is such that another 7-10 years operation at an internationally recognized high level can be achieved without the requirement for major investments.

- User groups are based at all the major Dutch and Flemish universities and stimulate collaborations between these groups and internationally recognized high level research groups.

- The beamlines cover a very wide range of research fields but are especially an important research tool for Dutch, Flemish and high quality international research groups in the fields of catalysis, polymer and colloid research. There is a growing interest in the use of the beamlines by groups working with 'energy' related materials as well as environmentally relevant soil research.

- The beamlines are internationally recognized as being at the forefront of the development of simultaneous technique combinations.

- The main problem is the shortage of user support staff and this issue should be urgently addressed.

1 Introduction and brief history

1.1 Introduction

The Dutch Belgian Beam Lines at the ESRF (DUBBLE) project is a shared initiative between the Dutch and Flemish research councils (NWO/FWO) to operate two beamlines at the European Synchrotron Radiation Facility (ESRF). The remit is to provide experimental possibilities for the Dutch and Flemish research communities in addition to the beam time that is available to the Dutch and Belgian researchers via the BENESYNC participation in the central ESRF laboratory. The beam lines have been in operation for about 10 years and in this period produced data which have been used in more than 500 refereed publications and over 100 PhD theses as well as formed the basis for several patents.

The core funding of DUBBLE is an operations budget that is provided on a 75:25, NWO/FWO basis and the beam time is, in this ratio, made available to Dutch respectively Flemish user groups.

The beamlines are specialized in two techniques for which the ESRF, via the public beam line access program, cannot provide sufficient access to satisfy the Dutch and Flemish demands. The two main techniques are combined Small and Wide Angle X-ray scattering (SAXS/WAXS) and X-ray absorption spectroscopy (XAFS). A minor amount of the available experimental time is used for Interface Diffraction (ID). There is a strong emphasis on time-resolved experiments and the simultaneous combination of different techniques. The latter are not necessarily X-ray based but, when required, can also encompass techniques which provide thermodynamic or chemical information. Intrinsic to this type of time-resolved experiments is the requirement to be able to utilize on-line sample environments that can perturb the samples homogeneously under well controlled conditions. The DUBBLE beamlines are well equipped to be able to handle this type of sample handling equipment.

In the coming years there will be changes at the ESRF. For the first time in its existence the budget has been reduced with a consequent closure of some of the public beamlines. At the same time a 5-7 year upgrade program is taking place. Apart from being able to deliver only 50% of the normal amount of beam time in 2012, there are no immediate consequences for the operation of the DUBBLE beamlines, since these are funded separately from the ESRF budget. It can be expected that the publication output from both the public- as well as the DUBBLE beamlines will temporarily decrease.

Although not strictly within the remit of the DUBBLE review some facts of the Benesync use of the public ESRF beam lines are included in appendices.

1.2 Brief history

NWO has a long history of participation in Synchrotron Radiation (SR) laboratories. This started over 30 years ago in the first facility dedicated SR user facility in Daresbury. When the new ESRF was constructed Belgium and the Netherlands decided to form a consortium to participate as equal partners for a total of 6% in this new facility[1].

The collaboration between NWO and FWO regarding the construction of two beam lines at the ESRF started in 1987. The beamlines were designed and constructed in close collaboration with the drawing offices and workshops of AMOLF and NIKHEF. The first beam line started generating experimental results in 1999 followed by the second in 2003. Originally it was foreseen to implement 4-5 experimental techniques. Due to technological developments, user pressure for different techniques and a gradual changes in the research landscape in the Netherlands and Flanders it was decided to limit this to two main techniques (SAXS/WAXS and X-Ray spectroscopy) and one minor (Interface Diffraction).

Previous project reviews have taken place in 2002 (5 yearly ESRF review) and 2007 (5 yearly ESRF review as well as an NWO/FWO initiated review). The self assessment documents and review panel reports can be found on the accompanying disk.

[1] The minimum participation for a full member was set at 4%.

2 Mission, Objectives and Vision

2.1 Mission

The core mission of the DUBBLE project is to provide synchrotron radiation beam time for the Dutch-Flemish research community in experimental techniques which are not sufficiently available via the participation in other synchrotron radiation laboratories, particularly the ESRF. The experimental facilities offered to the research community should be of a high qualitative level.

2.2 Objectives

The objectives of DUBBLE are :

- provide 70% of the available experimental time to the Dutch-Flemish user community
- provide 30% of the available experimental time to the international community
- provide experimental facilities at an internationally recognized high level
- provide a low threshold access for Dutch and Flemish users

2.3 Vision

An efficient and high level of experimental opportunities should be offered to the users thus enabling a large scientific output at an internationally recognized qualitative high level.

The beam lines are continuously developed driven by interplay of user demands, novel technological developments and imaginative use of combinations of existing technologies. The scientific staff, with the broader oversight of both the multidisciplinary scientific demands as well as the technological possibilities, fulfils a pro-active role in this process.

In the 30% of the international beam time it is aimed to attract and retain a user base of high level international user groups and stimulate collaborations between these user groups and the Dutch-Flemish community.

3 Organisation

3.1 Administrative

The administrative organisation of DUBBLE is given in diagram 3.1. The overall structure has remained unchanged since the previous reviews even though the way that the different positions in the Steering committee are being filled has changed as well as the role that the Program committee is supposed to play. These changes will be discussed in the chapter on developments.

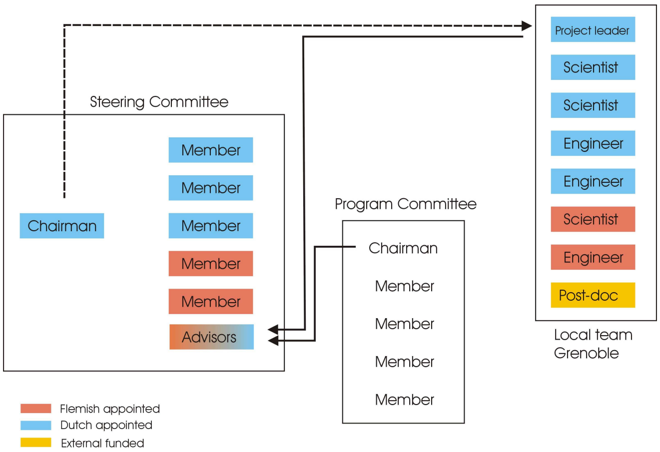

Figure 3.1 Block diagram of the administrative organization of DUBBLE

The chairman of the steering committee is the formal representative of DUBBLE to the ESRF. NWO is the legal contracting party to the ESRF.

3.2 Operational organization

DUBBLE is a Collaborative Research Group (CRG) at the ESRF. This means that 70% of the experimental time (beam time) is made available for research groups within the remit of the funding agencies NWO and FWO. These research groups are either university or national research laboratories (e.g. FOM/IMEC) based. Access is also available for private/semi-private research laboratories under the condition that the data is published in the open literature. The 70% of the available beam time is on a time-averaged basis divided in 75% NWO and 25% FWO in proportion to the financial contributions from the funding agencies.

The remaining 30% of the beam time is, according to ESRF regulations, made available to general ESRF users. These user groups are in general European based.

Dutch and Belgian users also have access to the ESRF public beam lines via the Benesync consortium. This provides access to a larger portfolio of techniques. The overall share of 6% to which Benesync users are entitled is at present not fully used although the beamlines that offer comparable techniques to DUBBLE are also for the full 6%, or more, used by Dutch and Belgian users.

3.3 Access to the facility

Access to beam time is regulated differently for the 70% of CRG beam time and the 30% ESRF beam time. The ESRF has implemented a large system comprised of several committees with specific expertise in certain research fields. These committees meet twice a year in Grenoble and provide the ESRF directorate with a prioritized list of beam time applications based upon scientific relevance. The ESRF directorate then applies a distribution algorithm to ensure that the participating countries are allocated a share in the available beam time proportional to their contributions to the ESRF budget. The 30% of DUBBLE beam time that has to be made available to the ESRF is regulated by the above described process.

For the 70% private beamtime a different process is followed. A set of 4 referees, appointed by the steering committee of DUBBLE, provides a prioritized list. These referees are supposed to asses all proposals and they are not allowed to apply for beam time at DUBBLE. The referees are not in direct contact with each other[2]. The DUBBLE program committee subsequently can suggest (motivated) changes in the priority list. The final decision is taken by the steering committee. In principal the ranking is on scientific merit. However, research groups whom apply for the first time are in general granted their beam time.

For both the ESRF as well as the CRG share of the proposals a technical assessment is made in which the experiments are scrutinized for their technical feasibility. To some degree this assessment is taken into account by the referees and the controlling bodies.

For neither the public nor the private beam time allocation procedure a feedback mechanism, in which past publications based upon earlier received beam time are taken into account, is used.

With the Swiss-Norwegian CRG at the ESRF there is an exchange agreement in which a limited amount of beam time on their powder diffraction, single crystal diffraction and combined Raman/XAFS set-ups can be used in exchange for access to the DUBBLE facilities for their user community.

3.4 The local team

The staff in Grenoble maintains, operates and develops the beamlines and provides user support in the broadest sense. This ranges from establishing contacts with potential new user groups, investigate technique improvements, discus the scientific issues with the users, help and train users in data analysis and find user groups in hitherto unexplored research areas etc.

There is no differentiation between user support for international ESRF and 'CRG' users. Wherever meaningful the staff tries to initiate informal collaborations between the different groups using DUBBLE in order to benefit from the synergy off collaborating teams in shared expertise, financial resources etc.

[2] This is seen by some referees as a weak part in the procedure. In the view of the wide range of research subjects carried out on the beam lines it is impossible that the referees are familiar with all of these and it should be possible to compare confidence levels in the assessments.

Each of the scientific staff members is involved in research activities as well. This both via the in-house research program but as well as via collaborations with user groups.

Although not part of their remit the local team is also often assisting new or potential user groups to identify which ESRF public beam line is providing the best solution if experiments require techniques that cannot be carried out on DUBBLE and mediate in the contacts with other beam line scientists.

4 Technical

A brief technical description of the beam line optics is given in Appendix 1. More detailed descriptions can be found in the previous reviews which can be found on the accompanying disk.

4. 1 Radiation source

The public ESRF beam lines are nearly all developed around undulator magnets. For some techniques this is crucial since these beam lines offer a higher flux and a higher collimation. However, for techniques that are detector, instead of flux, limited or where a continuous photon spectrum is beneficial, the bending magnets are equally well suited or better.

The radiation sources for the beam lines are the 0.4 T bending magnet spectrum for the XAFS beam line and the 0.8 T spectrum for the SAXS/WAXS line. The working energy range as specified in the original concept was for both beam lines from 5-30 keV. This is still the case for the SAXS beam line but in response to used demand it has been extended from 4- 42 keV for the XAFS beam line.

4.2 BM26A/XAFS beamline

For non-energy dispersive XAFS the continuous energy spectrum of a bending magnet is preferable over the peaked undulator spectrum. This beamline has a flux of around 10^{11} photons/sec which in the normal operation mode can be focused in a 300 micron spot. It is possible to perform transmission, fluorescence and electron yield spectroscopy. Also a confocal microfocus option has been implemented and it is possible to perform tomographic XANES and micro-fluorescence experiments with a beam size of 10 microns or less. Especially the first option is unique at the ESRF and limited available in other laboratories.

A gas handling system for operations up to 30 Bar under controlled flow conditions has been installed and is available for catalysis and hydrogen/CO_2 storage experiments.

The strong points of this station are the very high level of the available experimental infrastructure and the possibility to combine several other X-ray techniques with X-ray spectroscopy. Especially the combined SAXS/WAXS/XAFS set-up deserves to be mentioned since this is at present unique. This set-up renders in a single time-resolved experiment information on the chemical state of materials as well as structural information over a range of 0.2 -100 nm.

After 6 years operation the data acquisition soft/hardware is in need of a major overhaul. The contract for this has been signed and the software will be installed in 2011. The new software is less PC platform dependent and will also allow easier interfacing to new detectors and sample control PC's.

This beam line receives on average 1-2 visiting research groups/week.

4.3 BM26B/SAXS/WAXS beamline

In the normal operation mode the SAXS/WAXS beamline generates a flux of 10^{11} photons/sec in a 300 micron spot. Diffraction distance from 0.15- 200 nm can be resolved. Time-resolved experiments can be carried out down to a msec/frame thanks to the recent upgrades with two photon counting Pilatus detectors. The beamline was designed to be able to install large scale sample handling equipment in order to follow for instance polymer processing techniques on-line.

Two post-focusing microfocus systems are available. A low background Kirkpatrick-Baez system which generates a spot size of 12 microns with a low angle resolution of 50 nm (real space) for soft condensed matter experiments. The flux is around 10^{10} photons/sec. The second is a microfocus Compound Reflective Lenses (CRL) which is used extensively for the studies of silica based colloidal systems (Lekkerkerker, Utrecht). This focus the beam down to around 10 microns. The latter option preserves the beam coherence and allows diffraction distance of 1 micron to be studied at the expense of a somewhat elevated background.

The data acquisition software has recently been upgraded to the GDA system developed at the Daresbury/Diamond laboratories. This standard has now been adapted on SAXS beamlines at Diamond, the APS and ALBA (instigated by DUBBLE staff).

The strong point of this beam line is the ease with which both large and small scale sample environments can be mounted.

The beam line has been in operation since 2000. After the recent detector and software upgrades this beamline has confirmed its status as belonging to the top category of materials science X-ray scattering beamlines.

In this experimental hutch also an Interface Diffractometer (ID) is installed.

This beamline receives on average 2 research groups/week.

5 Staffing

The Dubble team consists of one projectleader and three PhD level beam line scientists. In addition there is an externally funded postdoc position. Apart from the project leader all scientists have a user support role and beam line development task. Besides this there is a limited possibility for own in-house research. There are different employment routes. Either via NWO or via Flemish universities or locally. A third employment route is via the ESRF where the combined CRG's are funding several posts relating to administration, mechanical technical, electronic technical and software support. This provides access to a variety of skills that are only occasionally required.

The main activity at DUBBLE is user support and beam line development. The user support is carried out by persons at PhD level and is in table 5.1 indicated by 'research staff'.

At present there is one PhD student funded via University College London (Bras/Sankar/Catlow collaboration. This student should finish in September 2011 and a new student has been recruited as successor. For the last 7 years a postdoc position has been funded by the Dutch Polymer Institute (DPI). This terminates October 2012. The recruitment procedure for a 2 year postdoc via the Alistor network has started.

With this staff 2 beamlines are operated on a 24 hours, 6 day/week schedule.

	2007	**2008**	**2009**	**2010**	**2011**
Tenured staff	1	1	3	3	3
Non tenured staff	4.16	4.16	2.16	2.16	2.16
PhD students			1	1	1
Total research staff	**5**	**5**	**6**	**6**	**6**
Technical staff	3	3	3	3	3
Visiting fellows		0.5	0.5	0.5	0.5
Staff via ESRF	0.6	0.6	0.6	0.6	0.4
Total staff	**8.76**	**9.26**	**10.26**	**10.26**	**10.06**

Table 5.1 staffing levels period 2007-2011

The personnel at present:

Dr. W. Bras

Project leader, overall responsibility, instrumentation development (both optics as well as sample environments and technique combinations), attracting new user groups, contact with existing user groups about research directions. Carries out own research and supervises the research from the team members and the students/postdocs. Spends 2 x 1 month/year in Lawrence Berkeley Laboratory

Ir. D. Detollenaere

Senior engineer, data acquisition electronics, computer support, vacuum specialist, supplier contacts

Mr. S. Nikitenko

User support XAFS, beam line operation, beam line scheduling, instrumentation development. Carries out own research.

Dr. G. Portale

User support SAXS, beam line operation, beam line scheduling, instrumentation development, polymer research. Carries out own research.

Dr. M. Silveira

Instrumentation development, User support XAFS. Carries out own research.

Dr. D. Hermido

DPI postdoc, DPI user support, Carries out own research.

Dr. L. Apostol

Data acquisition software maintenance and development, software/hardware interfaces, data analysis software, website

Mr. F. Ledrappier

Mechanical engineer, technical user support

Vacancy

Alistor postdoc

The visiting fellows:

Dr. Allessandro Longo

Palermo University. Involved in the technical development of GISAXS hard- and software

Dr. Jim Torbet

Free lance. Involved in biophysics projects. Teaching local staff about biological fibre diffraction

Dr. Rik van Deun

Use of EXAFS in coordination chemistry. Organisation EXAFS schools.

Dr. Roelof van Silfhout

Development of X-ray beam position monitors. This work has resulted in 5 publications co-authored with DUBBLE staff. This work has also resulted in a patent. Also a beam stabilization unit on BM26A was developed which uses a feedback loop between the beam position monitor and the mirror position. Regular consultant to DUBBLE on optical systems

Dr. Guy Luijckx

Replacement of the project leader for 2 x 2 weeks/year. Also contacts with engineering companies in Netherlands/Belgium.

Both W. Bras and D. Detollenaere have been involved in DUBBLE from the start. Most of the knowledge regarding the user base, overview research fields and optical design resides with W. Bras whilst most of the operational details of the beam lines are in the hands of D. Detollenaere.
In 2009 the NWO management realized that to retain competent staff it was required to convert two temporary posts to permanent which are taken up by S. Nikitenko and G. Portale. However, this has not alleviated another major problem which is the understaffing of DUBBLE. Only by relying on the willingness of the staff to support the users by working far in excess of the normal working hours is it possible to operate the beam lines. This is obviously at the expense of the scientific career development of the staff.

Staffing levels at ESRF beam lines, and most other SR sources, are considerably higher. The standard user support complement of an ESRF beam line is two scientists, two postdocs and a 50% beam line operations manager. This is approximately twice the amount of manpower compared to DUBBLE. With no extra user support staff the present level of support is not sustainable. Within the Dutch and Flemish grant system there is no suitable program where one can apply for personnel for user support. At present the DPI postdoc also assumes the user support role for DPI users. However, in the light of the financial situation of DPI one cannot be sure that this post will be continued beyond the second half of 2012.

In general it is difficult to recruit staff that can operate at the appropriate level. This is not unique for DUBBLE but is shared with most synchrotron radiation facilities. However, the problems at DUBBLE are aggravated due to the lack of career structure, higher workload and salary scales.

6 Financial

DUBBLE is financed through a collaboration between NWO and FWO. The financial administration is carried out by NWO. There are two noteworthy points:

- within NWO the DUBBLE budget was traditionally linked to the ESRF and ISIS participations. Only recently this has been disentangled and some clarity obtained
- early in the existence of DUBBLE it was found that the Flemish personnel overheads were substantially larger compared to the Dutch system. At that moment it was decided that the Flemish funded personnel administratively would be handled separately.

Evaluatie DUBBLE baten en lasten	**2007**	**2008**	**2009**	**2010**
Loon- en prijsbijstelling DUBBLE 2007		3.7	3.7	7.1
Loon- en prijsbijstelling DUBBLE 2008		8.4	8.4	16.2
Loon- en prijsbijstelling DUBBLE 2009			4.1	7.8
Bijdrage NWO tbv DUBBLE (AB 410)	0.0	798.0	480.0	480.0
Aanvulling bijdrage NWO 2008 tbv DUBBLE (AB 410)		280.9		
Baten NWO	**0.0**	**1,091.0**	**496.2**	**511.1**
Bijdrage FWO DUBBLE	137.8	120.3	138.1	220.8
Overige baten			30.0	11.5
Bijdragen derden	**137.8**	**120.3**	**168.1**	**232.3**
Bijdrage CW		96.0	225.0	225.0
Bijdrage CW				304.0
Bijdrage N		96.0	225.0	225.0
Bijdrage STW		3.0	30.0	30.0
Interne bijdragen	**0.0**	**195.0**	**480.0**	**784.0**
Investering Chemie plus matching DUBBLE (K€25)				329.0
Totaal baten	**137.8**	**1,406.3**	**1,144.3**	**1,527.4**
Salariskosten	304.9	404.6	364.8	347.2
doorberekende salariskosten	-152.8	-65.9	-14.3	0.0
Salariskosten derden	63.3	50.0	127.2	73.5
Reiskosten buitenland		40.1	12.3	24.1
Overige kosten	14.9	19.2	58.7	55.2
ESRF servicekosten	540.9	499.8	575.4	602.0
Investering Chemie plus matching DUBBLE				133.8
Lasten Dubble Grenoble	**771.2**	**947.8**	**1,124.1**	**1,235.8**
Beurzen	55.8	44.6	58.2	63.2
Overige kosten				2.0
Lasten Dubble via NWO	**55.8**	**44.6**	**58.2**	**65.2**
Totaal lasten	**827.0**	**992.4**	**1,182.3**	**1,301.0**

Table 6.1

Expenditure DUBBLE beam lines according to NWO financial administration for the period 2007-2010.

(Data provided by Agnes van den Broek, NWO)

The post ‘ESRF servicekosten’ are in fact the local costs incurred in Grenoble via the ESRF administration. These are billed quarterly to NWO. However, this is staggered in time with the last quarter of year *N* billed to NWO in year *N+1*. A part of this consists of real service costs (energy, fluids, gasses etc.) but also the collectively hired CRG manpower is part of this. In table 6.2 the fixed annual costs are given.

	k€	
personnel	45	Secretarial, technical, software engineers, lab technician
services	23	Electricity, water, liquid nitrogen etc.
insurance	8.4	Compulsory equipment insurance
computing	11	Data storage, network, licenses
mechanical	7	Handling, alignment, access workshops
various	7	Cleaning etc.
total	**101.4**	

Table 6.2 Annual fixed costs incurred locally in Grenoble via the ESRF administration

After the 2007 reviews it was decided to invest in equipment in order to bring the beamlines in a position that they would be suitable for another 10 years of high level operations. The spending profile for the major investments is given in table 6.3

	2007	2008	2009	2010	2011
Pilatus 300k		60	117		
Electron yield detector			14	1	
High pressure gas system*			100 (-30)		
DAQ software			47	50	
Pilatus 1M**				220	114
		60	248	271	114

*the gas system was partially financed by user groups

**the Pilatus 1M detector was obtained via the NWO-CW Middelgroot program (25% matching via DUBBLE budget)

Table 6.3 Major equipment investments in period 2007-2011

Since the start of the project in 1987 the budget has not significantly changed and has not been indexed for inflation. So far this has not been problematic but it can be foreseen that with several more years of operation this could become problematic.

Outside funding in the form of manpower is in general based upon collaborations of the project leader with University groups. So far DUBBLE has had the benefit of 7 postdoc years DPI, 2 years Eindhoven/Sheffield, 2 years Alistor network. Also 2 x 3 years of PhD funding via University College London.

7 Developments 2007-2011

7.1 Technical developments

The main optical equipment (monochromators and focussing mirrors) has been working satisfactory and there are no immediate plans for major modifications. The only intervention that is foreseen is the mounting of the collimating mirror on BM26A. This will take place in the first long, 'upgrade' associated, ESRF shutdown (First quarter 2012). All equipment and parts are available and this operation will be cost neutral. It will result in an increase in flux since the accepted solida angle of the radiation cone will be larger. Also a minor improvement in energy resolution is foreseen. Technical details of the beam lines can be found in Appendix 1 and in the review reports on the accompanying CD.

7.1.1 BM26A/XAFS

The experimental table has been upgraded in order to be able to handle more complicated and heavier sample environments. Also the changeover time between conventional XAFS and combined XAFS/diffraction/scattering experiments has been reduced considerably.

This new table has also allowed the introduction of polycapillary microfocus optics which have been used for microfocus XAFS[1] Confocal microfocus tomography has been developed by the group of L. Vincze in collaboration with DUBBLE staff. A focal spot of 10 micron has been achieved[3] and not only fluorescence data but also real XAFS data has been collected. This microfocus for the use of XAFS is rather rare at the ESRF and worldwide.

The second major upgrade has been the installation of a gas mixing system which allows catalysis based experiment to be carried out under flow and at high pressure. The system has been developed in consultation with several user groups whom also have co-funded this project (Weckhuysen, Utrecht; Hensen, Eindhoven; Haije, ECN).

The SAXS/WAXS/EXAFS facility has been further developed and is now routinely used by several user groups[2, 3].

The station has been equipped with a beam position monitor and positional feedback system to the focussing mirror. This results in a beam positional stability of around 2 micron. (system developed R. van Silfhout/DUBBLE)

An electron yield system has been used in the framework of the PhD work of Vladimir Martis. The specialty in this system is that it is possible to detect the electrons energy sensitive so that one can in a single experiment determine the EXAFS spectra generated at different depths below the surface. This system will be further developed for utilization with Li based batteries and electrochemistry in general. This will be done by the postdoc funded by the Alistor network. However, there are several other fields where this electron yield detector could be used.

[3] Nominal beam size is 0.3 x 1 mm^2 (VxH)

Figure 7.1

The new gas mixing system for catalysis research on BM26A

In the course of 2011 new data acquisition software will be installed which is not dependent anymore on the Sun workstations which at the time of installation (2004) were the ESRF standard but are now hardly maintainable.

Since 2007 this station has seen an increase in geochemical experiments related to soil contamination (Wageningen, Utrecht, Gent, Diepenbeek) as well as energy related research (CO_2 storage, H_2 storage and battery materials).

A slightly worrying, although not immediately threatening, problem is the state of the 9 element monolithic Ge detector for fluorescence measurements. This detector is ageing and the manufacturer refuses further maintenance. In the coming 2-3 years a decision has to be made about how to replace this detector. It should be stressed that this detector still delivers superb data quality.

At present this station represents a state of the art beam line with infrastructure specifically tailored for the Dutch-Flemish user community which also is much in demand with the general ESRF user group.

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7.1.2 BM26A/XAFS future developments

At present there are several studies about possible improvements/extensions to the BM26A station under investigation.

- the position sensitive Inel detector has a limited spatial resolution and is inefficient at higher photon energies. At present we're testing out an improvised powder diffractometer for time resolution. If these tests are successful this will be implemented in a more permanent fashion in the 2012 shutdown.

- in order to increase the time resolution of the experiments it could be considered to implement a fast scanning monochromator (Frahm type). However, this will have major consequences for the already existing optics and will require outside funding.

- in the light of the many studies that are taken place on both BM26A/B on the onset of crystallization in various systems (polymers, zeolites, bone mineralisation etc.) it might be interesting to invest in the possibility to make PDF scattering experiments possible. This technique can shed light on the amorphous/poorly crystalline state of very small clusters of atoms. However, it will be required to extend the energy range of the station to around 60 keV. This will require a reconstruction of the present monochromator as well as a major modification to the frame work of the experimental hutches. This would require major external funding.

- the gas system for XAFS should be extended with a mass spectrometer for measuring the output during on-line catalysis experiments. This probably can be taken care of within the DUBBLE budget with possibly a contribution of interested user groups.

- the major issue at present is the replacement of the Ge fluorescence detector. At present the idea is to obtain a Vortex Si detector for energies up to 20 keV and a 13 element Ge detector for the higher energies. A first attempt to obtain external financing will be via the NWO Bazis program (estimated 250 k€ required).

The user community of the XAFS instrument is slowly growing and becoming more productive. The interest in geochemical (environmental pollution) and energy storage materials is increasing. Also the demand in the catalysis community is still growing and XAFS is a workhorse technique in this for the Netherlands and Belgium industrially important activity. Worldwide there is a shortage of XAFS beamlines at present. It can be predicted that there will not be a shortage of high level research groups who require access to this type of experiment.

7.1.3 BM26B / SAXS

A new Pilatus 300K WAXS detector has been obtained with funds available in the operations budget. A second Pilatus detector (1M) has been obtained for the SAXS experiments. The funding for this has been provided by the NWO Middelgroot program. These two state of the art detectors are more sensitive (≈ 7x) and have a higher count rate limitation (10-100x) compared to the previous generation of detectors but still retain the single photon counting options which are important in low electron density contrast scattering experiments.

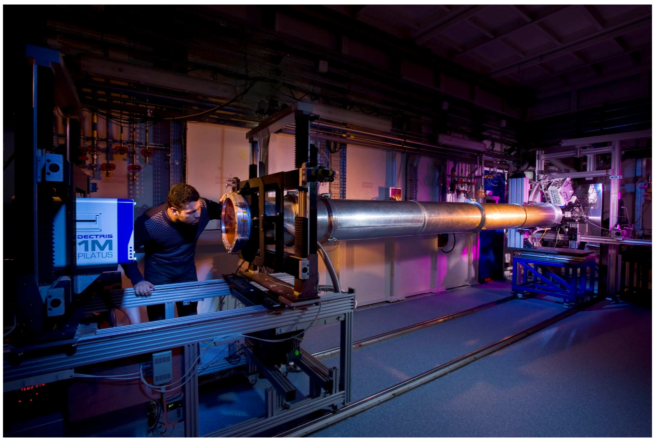

Figure 7.2

The SAXS/WAXS beamline equipped with the two new, state of the art, Pilatus detectors

In the March 2011 shutdown a translation system for three different optical systems will be installed in the experiments hutch. This makes it feasible to reduce the installation time of the two microfocus options from over a day to around 2 hours.

After 10 years operation new data acquisition software has been installed that is less platform dependent and from which the code is open source. This ensures maintainability as well as allows new sample handling equipment to be interfaced to the data acquisition software.

One of the weak points in SAXS is the (worldwide) lack of data analysis software other than for biological solution scattering. To partially remedy this DUBBLE staff has teamed up with Prof Stephan Förster (Bayreuth) and developed software suitable for the analysis of time-resolved anistropically scattering systems. This has been released to the user community[4].

Grazing incidence SAXS (GISAXS) experiments have been developed. This will be further developed by using the ID diffractometer which has the required accuracy for the reflection data that also have to be obtained when performing GISAXS experiments. The new photon counting Pilatus detector will make it possible to carry out anomalous SAXS experiments (ASAXS).

With the recent detector upgrades the SAXS set-up is ready for another 10 years of operation at top level.

The Interface Diffractometer has been hardly used in the last three years. The two user groups using this diffractometer were not very successful with their beam time applications, have applied less and have also been able to obtain beamtime on the specialised ESRF undulator lines which have an intrinsic higher flux beneficial for these experiments. No publications have appeared from this instrument since 2008.

Section Reference

4. Forster, S.; Apostol, L.; Bras, W., Scatter: software for the analysis of nano- and mesoscale small-angle scattering. *Journal of Applied Crystallography 43*, 639-646.

7.1.4 BM26B / SAXS future developments

- Thanks to improvements in block-copolymer synthesis many functional systems have become possible to fabricate. For instance applications as solar cells and sensors require materials to be self assembled in thin films. In order to follow this process grazing incidence SAXS (GISAXS), and reflectivity, is required. The further development of this equipment is in progress.
- There still remain large issues with data analysis software for SAXS. This will be tackled by porting the existing Scatter software to a more convenient platform (Java or Python). This will be done in collaboration with the Diamond and APS SR laboratories.

The user community of SAXS/WAXS ranges over a very wide range of research fields, especially relevant in nanotechnology, with several fields still unexplored due to lack of available beam time. There is no reason to assume that the average number of research groups will drastically alter although the composition of the user community slowly evolves in time. Therefore we can predict that the requirement for access to a high level SAXS/WAXS instrument will remain high within at least the coming 10 years.

7.2 User developments

7.2.1 Users by geographical distribution

The Dutch-Flemish user community is rather stable with slow changes and increase in number through the years. The increased experience of groups has a positive effect on publication output which is steadily increasing. The geographical distribution among the universities is such that Eindhoven and Utrecht University make up the largest number of user Dutch groups but that nearly all other universities are represented as well. Recently the use by Delft based groups has increased. The largest number of Flemish research groups using DUBBLE can be found in Gent and Leuven. An overview of the different groups can be found in Appendix 2.

The user groups that make use of the ESRF part of the beam time is geographically widely distributed. Around 50% of these groups have research collaborations with Dutch or Flemish groups. Most of these are internationally highly rated groups and are involved in the more complicated experiments. The other 50% is made up of users that require access to a relative simple set-up which can be provided by any SAXS or XAFS station.

7.2.2 Trends in research directions

The main research subjects have remained unchanged. As predicted in 2007 the percentage of publications related to EXAFS has sharply increased. This is due to the fact that in the previous review period the EXAFS station had only become operational two years earlier whilst in the 2007-2011 review period this station was fully active. The relative decrease in polymer related publications should be seen in the light of the increased output. The absolute number is hardly changed (around 100 publications in both periods). Growth can be seen in geochemistry and energy materials. Also an increase in metals and alloys research is seen in the beam time proposals. However, this is a recent trend and does not show up in the publication output yet.

In figure 7.3 the percentage of publications in different research fields is shown and a comparison is made with the situation in 2007.

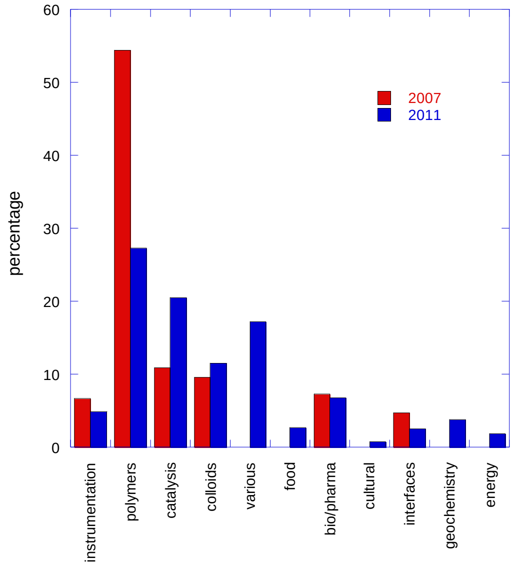

Figure 7.3

Development of the main research areas targeted by the DUBBLE user group

The degree of sophistication of the experiments carried out on both BM26A as well as BM26B has increased with more emphasis on technique combinations in the case of BM26A and more complicated sample environments on BM26B. Most of these complicated experiments are hardly possible on ESRF stations nor anywhere else. This is partially due to the expertise and involvement of the DUBBLE staff and partially due to lack of the required infrastructure on other beam lines. Most of this infrastructure is developed by the DUBBLE staff in consultation with the Dutch/Flemish user community.

7.3 Training

After a sabbatical that Dr. R. Van Deun has spent at ESRF/DUBBLE it was realized that it would be very beneficial for the relative inexperienced Flemish user community to organize EXAFS data analysis courses. These courses were organized in 2010 (entry level, 50 attendants) and 2011 (advanced level, 25 attendants) This was co-organized by Drs R. Van Deun, G. Silversmit and DUBBLE staff. The audience was from both Flanders as well as the Netherlands.

For 2011/2012 a similar initiative is foreseen for SAS. This will be co-organised by Drs. W. Bouwman (SANS), W. Bras (SAXS) and E. Polushkin (lab source based SAXS). Panalytical (Almelo) has also expressed an interest in participating in the organization.

It would be beneficial if the knowledge of the techniques that are used at DUBBLE would be further spread. One way to achieve this is by the courses as mentioned above but another option could be to create 2-3 month fellowships in which senior university (permanent) staff would be based in Grenoble to familiarize themselves with the techniques and data analysis methods. In this way the knowledge base could be extended[4].

[4] In the light of the underuse of the ESRF this could be contemplated for the public beam lines as well.

7.4 Governance

Since 2007 the governance structure of DUBBLE has changed. In the old structure the Stuurgroep was composed of senior university professors with broad expertise in their research field and acquainted with the techniques and research fields of DUBBLE. Since the internal financing structure for DUBBLE in NWO has changed the Gebiedsbesturen have asked for more influence and in the new structure representatives of the Gebiedsbesturen are members.

The remit of the Program Committee has changed and attempts have been made to broaden the tasks of the committee. In the old situation the program committee assessed the beam time proposals and discussed the developments with the project leader. The steering committee had to approve the ranking of the proposals. In the new structure the idea from NWO-side was that the program committee would be responsible for long-term developments within DUBBLE, the finances and a broadening of the user group. (This was in the old situation the remit of the project leader). The ranking of proposals is carried out by external referees. Besides this, it was hoped that the committee would function as a Dutch advisory board for the use of synchrotron radiation in the broadest sense.

The self assessment of the Program Committee was that the expertise, insights in the daily operations and overview over the technical aspects of synchrotron radiation was not sufficient to fulfill all the set tasks especially with regard to advice in the broadest sense since all members were chosen in the Program Committee because of their specialist expertise relevant to the DUBBLE beamlines. Moreover, it highly overlaps with the work of the project leader, who has much more insight in all aspects of the beamline operation and a broader overview of the scientific community using DUBBLE as well as the ESRF.

At present it is not clear to all involved what the relations between the different participants is.

This paragraph has been read and approved by Dr. Han Goossens, chairman of the Program Committee during the transition period.

8 Representative publications

References to representative publications with data from the DUBBLE beamlines are shown below. It is chosen to show publications per technique with a predominantly Dutch or Flemish author list as well as references to work by international users.

EXAFS

1. Nikitenko, S.; Beale, A. M.; van der Eerden, A. M. J.; Jacques, S. D. M.; Leynaud, O.; O'Brien, M. G.; Detollenaere, D.; Kaptein, R.; Weckhuysen, B. M.; Bras, W., Implementation of a combined SAXS/WAXS/QEXAFS set-up for time-resolved in situ experiments. *Journal Of Synchrotron Radiation* **2008,** *15*, 632-640.
2. Di Vece, M.; Bals, S.; Verbeeck, J.; Lievens, P.; Van Tendeloo, G., Compositional changes of Pd-Au bimetallic nanoclusters upon hydrogenation. *Physical Review B* **2009,** *80* (12), 4.
3. Beale, A. M.; van der Eerden, A. M. J.; Jacques, S. D. M.; Leynaud, O.; O'Brien, M. G.; Meneau, F.; Nikitenko, S.; Bras, W.; Weckhuysen, B. M., A combined SAXS/WAXS/XAFS setup capable of observing concurrent changes across the nano-to-micrometer size range in inorganic solid crystallization processes. *Journal Of The American Chemical Society* **2006,** *128* (38), 12386-12387.
4. Van Damme, A.; Degryse, F.; Smolders, E.; Sarret, G.; Dewit, J.; Swennen, R.; Manceau, A., Zinc speciation in mining and smelter contaminated overbank sediments by EXAFS spectroscopy. *Geochim. Cosmochim. Acta 74* (13), 3707-3720.
5. Bruggeman, C.; Maes, N., Uptake of Uranium(VI) by Pyrite under Boom Clay Conditions: Influence of Dissolved Organic Carbon. *Environmental Science & Technology 44* (11), 4210-4216.
6. Walspurger, S.; Cobden, P. D.; Haije, W. G.; Westerwaal, R.; Elzinga, G. D.; Safonova, O. V., In Situ XRD Detection of Reversible Dawsonite Formation on Alkali Promoted Alumina: A Cheap Sorbent for CO2 Capture. *Eur. J. Inorg. Chem.* (17), 2461-2464.

SAXS

1. Rissmann, R.; Groenink, H. W. W.; Gooris, G. S.; Oudshoorn, M. H. M.; Hennink, W. E.; Ponec, M.; Bouwstra, J. A., Temperature-induced changes in structural and physicochemical properties of vernix caseosa. *Journal of Investigative Dermatology* **2008,** *128* (2), 292-299.
2. de Wit, J.; van Ekenstein, G. A.; Polushkin, E.; Kvashnina, K.; Bras, W.; Ikkala, O.; ten Brinke, G., Self-assembled poly(4-vinylpyridine) - Surfactant systems using alkyl and alkoxy phenylazophenols. *Macromolecules* **2008,** *41* (12), 4200-4204.
3. Besenius, P.; Portale, G.; Bomans, P. H. H.; Janssen, H. M.; Palmans, A. R. A.; Meijer, E. W., Controlling the growth and shape of chiral supramolecular polymers in water. *Proceedings of the National Academy of Sciences of the United States of America 107* (42), 17888-17893.
4. van den Pol, E.; Petukhov, A. V.; Thies-Weesie, D. M. E.; Byelov, D. V.; Vroege, G. J., Experimental Realization of Biaxial Liquid Crystal Phases in Colloidal Dispersions of Boardlike Particles. *Physical Review Letters* **2009,** *103* (25), 4.
5. J. C. Gielen, M. Wolffs, G. Portale, W. Bras, O. Henze, A. F. M. Kilbinger, W. J. Feast, J. C. Maan, A. Schenning and P. C. M. Christianen, Molecular organization of cylindrical sexithiophene aggregates measured by X-ray scattering and magnetic alignment, Langmuir 25 (2009), no. 3, 1272-1276.

International users

1. Detlefs, C.; Duc, F.; Kazei, Z. A.; Vanacken, J.; Frings, P.; Bras, W.; Lorenzo, J. E.; Canfield, P. C.; Rikken, G., Direct observation of the high magnetic field effect on the Jahn-Teller state in TbVO4. *Physical Review Letters* **2008,** *100* (5).
2. Masciocchi, N.; Galli, S.; Colombo, V.; Maspero, A.; Palmisano, G.; Seyyedi, B.; Lamberti, C.; Bordiga, S., Cubic Octanuclear Ni(II) Clusters in Highly Porous Polypyrazolyl-Based Materials. *Journal of the American Chemical Society 132* (23), 7902-+.
3. Howse, J. R.; Topham, P.; Crook, C. J.; Gleeson, A. J.; Bras, W.; Jones, R. A. L.; Ryan, A. J., Reciprocating power generation in a chemically driven synthetic muscle. *Nano Letters* **2006,** *6* (1), 73-77.
4. C. Travelet, G. Schlatter, P. Hebraud, C. Brochon, A. Lapp, D.V. Anokhin, D.A. Ivanov, C. Gaillard, G. Hadziioannou, Multiblock copolymer behaviour of alpha-CD/PEO-based polyrotaxanes: towards nano-cylinder self-organization of alpha-CDs, Soft Matter, 4 (2008) 1855-1860.
5. N. Masciocchi, S. Galli, V. Colombo, A. Maspero, G. Palmisano, B. Seyyedi, C. Lamberti, S. Bordiga, Cubic Octanuclear Ni(II) Clusters in Highly Porous Polypyrazolyl-Based Materials, Journal of the American Chemical Society, 132 7902-+

9 Performance parameters

In this chapter the output and performance parameters of DUBBLE are discussed. For the performance parameters different ‘cross cuts’ have been made. Comparisons per technique, per similar organizational units and with the ESRF, in which DUBBLE is embedded, have been made.

9.1 Societal and economical impact

The societal impact of DUBBLE is hard to asses since for most research carried out at DUBBLE the intellectual property lies with the users. With respect to community outreach activities to the Dutch-Flemish the possibilities are unfortunately not very high. The travelling distance prevents most of the direct activities. Most Dutch-Flemish schools/student groups visiting the ESRF are received by members of the DUBBLE team (≈ 12 visits/year). Presentations regarding DUBBLE and the ESRF in general have been given at the annual NWO press day Bessensap, the Holland@CERN 2010 meeting and the Belgian crystallography meeting. Also journalists from het Chemisch Weekblad and their Flemish counterpart were invited.

The research carried out on DUBBLE ranges widely but encompasses societal relevant subjects like CO_2 and Hydrogen storage, development of eczema creams, cultural historical artifacts, soil contamination, polymer solar cells etc.

For proprietary industrial use DUBBLE is regulated by the ESRF standard conditions. This means that only a limited number of shifts is allowed to be sold at the rates dictated by the ESRF and that the ESRF is entitled to 25% of the revenue. Apart from Macromolecular Crystallography the sale of SR beam time in Europe is not widely spread and on DUBBLE limited to 1-2 days/year, mainly to Dutch or Belgian industries.

However, indirectly a large amount of the work done on DUBBLE is of interest to industries. At present there are two post doc positions financed by public-private organizations where industrial partners are part of the governing board. The Dutch Polymer Institute has founded a postdoc position for already 8 years. Recently the Alistor network approved funds to employ a postdoc working in Lithium battery materials.

More indirect industrial involvement can be seen from the large number of postdocs and PhD student whose positions are industrially funded. A comprehensive inventory is beyond the scope of this review but some examples can be given and can be found in Appendix 3. The information below is supplied by the named investigators. It should be stressed that this concerns non-proprietary research of which the results are published in the open literature.

From 8-11 September 2009 the Synchrotron Radiation and Polymer Science IV meeting was co-organized by W. Bras (DUBBLE), J.G.P Goossens (Eindhoven) and B. Goderis (Leuven) and attracted around 150 international participants. One of the goals of the organizers was to increase the Dutch and Flemish expertise and further stimulate international collaborations. The proceedings of this meeting can be found on http://iopscience.iop.org/1757-899X/14/1/011001.

9.2 Application pressure

The application pressure for both the ESRF to DUBBLE as well as from Dutch-Flemish users can vary considerably in time. In figure 9.1 the Dutch-Flemish and ESRF application pressure is given.

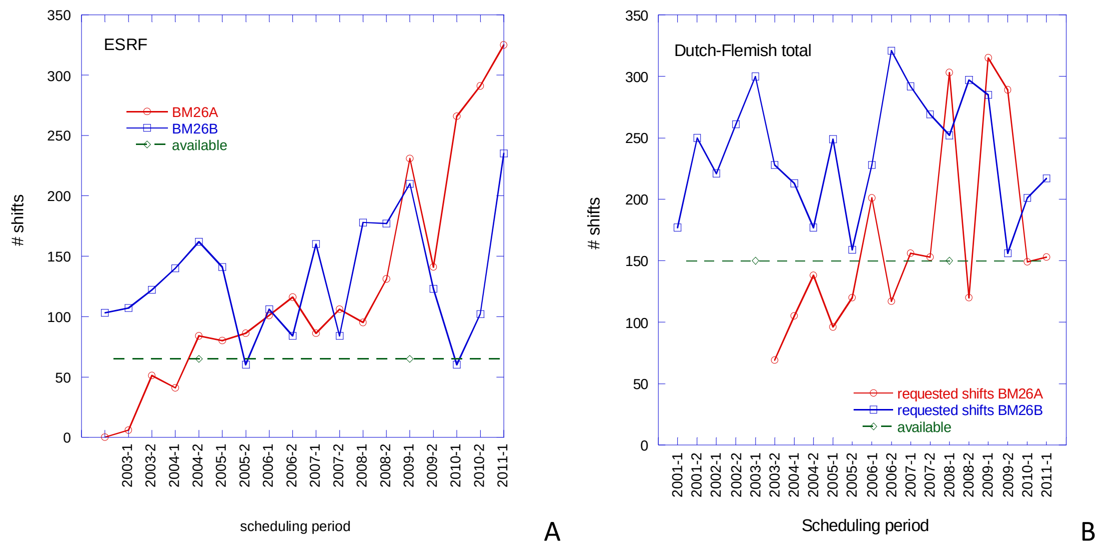

Figure 9.1 The application pressure on BM26A and BM26B. Panel 'A' the ESRF data (on average ≈ 65 shifts/six month period available). Panel 'B' the Dutch-Flemish requests (≈ 150 shifts/six month period available)

The recent large oversubscription for the ESRF part on BM26A is associated with the temporary closure of ESRF station BM29. The total oversubscription rate for both stations is manageable when the ratio remains between 1.5 – 2x. If the oversubscription increases above a factor 2x many users find the access too erratic in time and do not want to risk PhD/postdoc programs and consequently look for alternative beam lines or 'second best' techniques.

The number of shifts applied for and scheduled for the Dutch-Flemish community is given in figure9.2

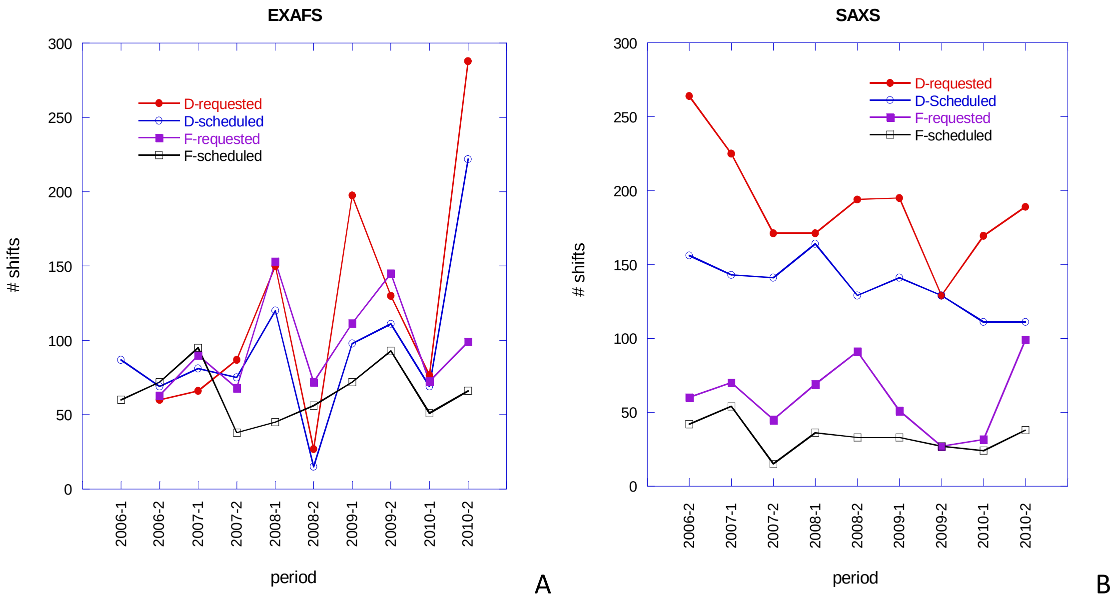

Figure 9.2
Applied for and scheduled shifts for Dutch and Flemish users. Panel A for BM26A and panel B for BM26B.

9.3 Delivered shifts

The ESRF is contractually obliged to deliver a certain number of user shifts/year. However, the accelerator complex is operating for a larger number of hours in different machine modes. Apart from the '4 bunch mode' all other machine modes are useable to the DUBBLE beamlines. On average DUBBLE should deliver around 650 shifts/year to the CRG users and around 280 shifts/year to the general ESRF users.

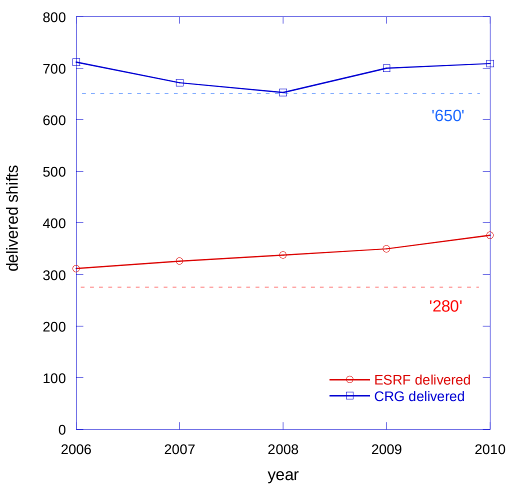

Figure 9.3 Number of shifts annually provided to users for BM26A and BM26B combined.

In general DUBBLE delivers more than is contractually required. It should be remarked here that this is favorable for the users but sometimes rather hard for the user support staff. Especially if one keeps in mind that DUBBLE is understaffed compared to the ESRF beam lines.

There is no data available on the reliability of the beamlines. Since the start of user operation only 1 – 2 user groups have received no useable data due to beam line failure (in 10 years time > 1000 experiments sessions have taken place). Occasionally there have been small issues with beam line vacuum or detectors. In general the ESRF accelerator complex has been very reliable as well.

9.4 Publication output

The annual publication output of DUBBLE is still steadily increasing[5]. See figure 9.4. It will be clear that this increase is not sustainable in the long run since ultimately one is limited by the amount of available beam time.

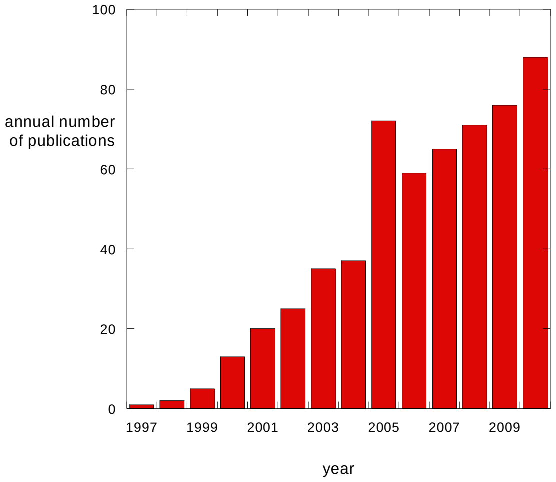

Figure 9.4

Annual number of refereed publications and PhD thesis with data from the DUBBLE beam lines.

In June 2010 the 500th publication appeared and Januari 2011 the 100th PhD thesis with DUBBLE data. The latter was work based upon a collaboration Eindhoven-Genua.

In this section we only deal with refereed publications and PhD theses. Since 2001 on average one article/year has appeared in, for instance, the annual ‘ESRF Highlights’. This type of material is not taken into account in this section.

[5] An up to date full list of publications is available at http://www.esrf.fr/UsersAndScience/Experiments/CRG/BM26/Publications

Figure 9.5 The bookshelf with thesis containing DUBBLE data.

Not only the number of publication is relevant but also the quality of the output can be measured to some degree. In figure 9.6 the percentage of publications as function of impact factor is given and compared to the situation of 2007.

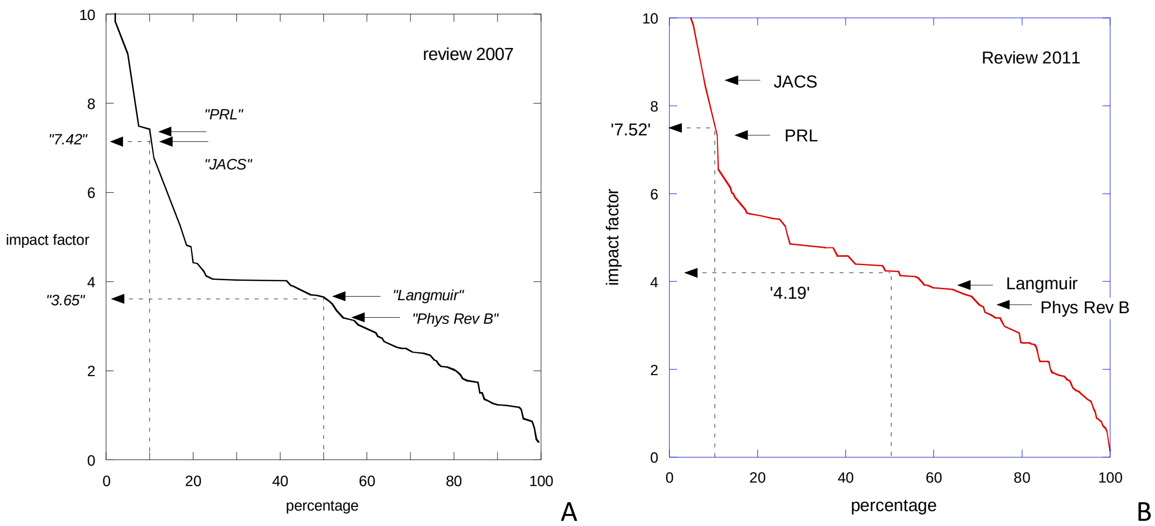

Figure 9.6
Percentage of publication (horizontal) with impact factors above a certain value (vertical). From this we can see that in 2011 10% of the publications appeared in journals with an impact factor above 7.52. Some relevant physics and chemistry journals are indicated.

From figure 9.6 we can conclude that the average impact factor has increased significantly. This can be partially due to variations in journal impact factors in time but probably the relative increase in catalysis papers compared to 2007 is partly responsible. These papers tend to be published in higher rated journals. The presence in the leading polymer research journal Macromolecules (impact factor 4.54) with 23 manuscripts remains high.

The relative number of manuscripts per research area has shifted somewhat. In figure 9.7 a comparison is made with the situation in 2007.

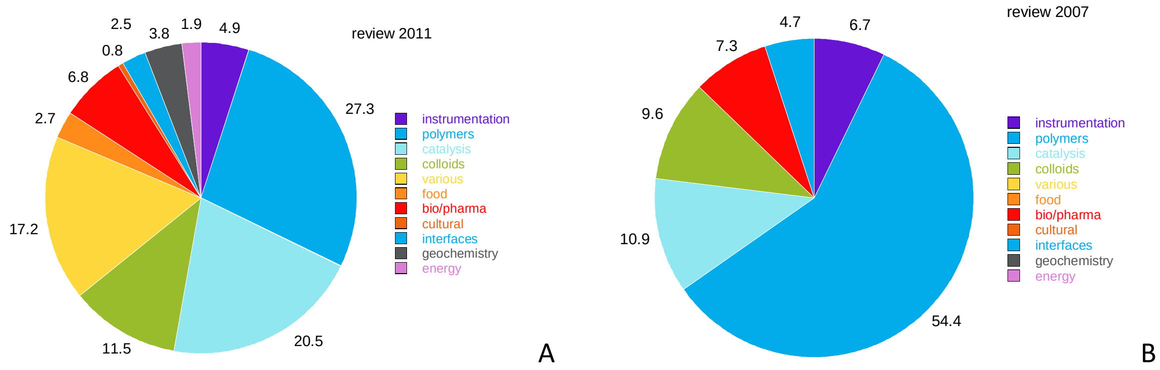

Figure 9.7

Percentages of publications in different research areas. Panel A shows the present situation and panel B the same in 2007.

We can see that the importance from catalysis has increased. However, one should keep in mind that in the previous review period the EXAFS station, which is used for much of this research, had only been on-line for a limited period. The categories 'cultural heritage' and 'geochemistry' were hardly represented in 2007.

For some of the most demanded techniques we have also shown the number of publications from Benesync users on ESRF public beamlines as well as on DUBBLE. See fig 9.8

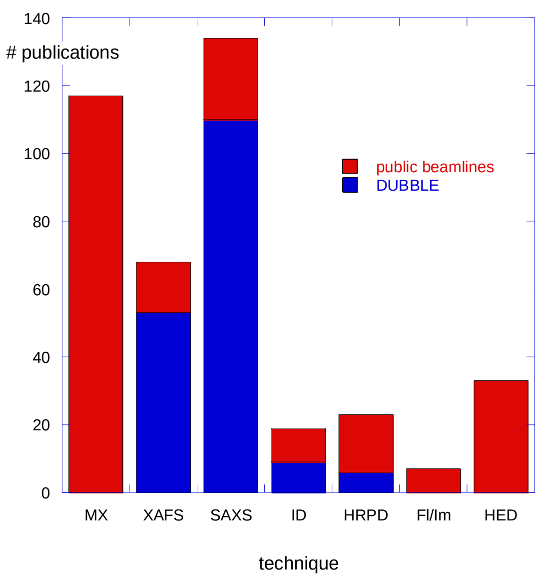

Fig 9.8 Number of publications per technique for DUBBLE (blue) and for Benesync users of ESRF public beamlines (red).

These results indicate that for the techniques that are available on DUBBLE the users also are successful in obtaining beam time in the open competition on ESRF public beam lines. This to the extent that they use up more than the roughly 6% of available public beamtime on these specific beamlines to which Benesync users are on overage entitled.

In figure 9.9 the total ESRF, Benesync and DUBBLE publication output is shown.

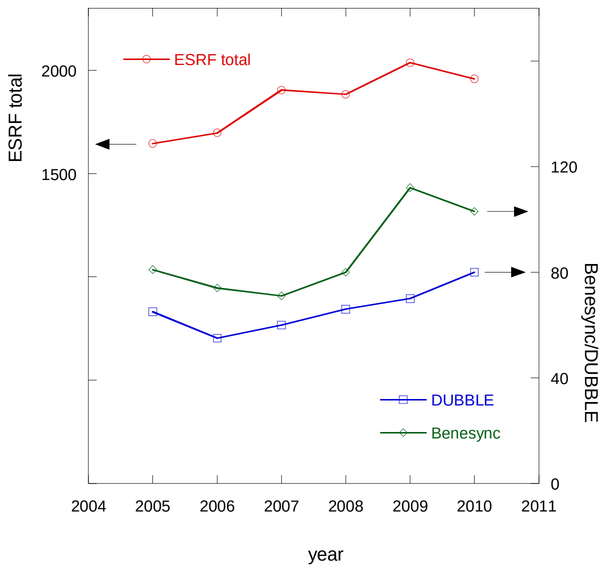

Figure 9.9
Publication output for the total ESRF (left hand scale) and DUBBLE /Benesync (right hand scale)

For the Benesync output it should be stressed that this concerns publications in which at least one co-author of a publication is based in a Dutch or Belgian laboratory. Further detailed research into this, if desired, is considered to be the responsibility of the research councils. It should be remarked that the annual Benesync contribution to the ESRF over the last years has been around 5.8% of 88 M€, i.e. ≈ 5.1 M€ and the annual costs for DUBBLE are around 1.2 M€. This indicates that the presence of a CRG at the ESRF is a very cost efficient way of maximizing the 'return on investment'.

The distribution of publications over the two main techniques between Dutch and Flemish laboratories is given in fig 9.10.

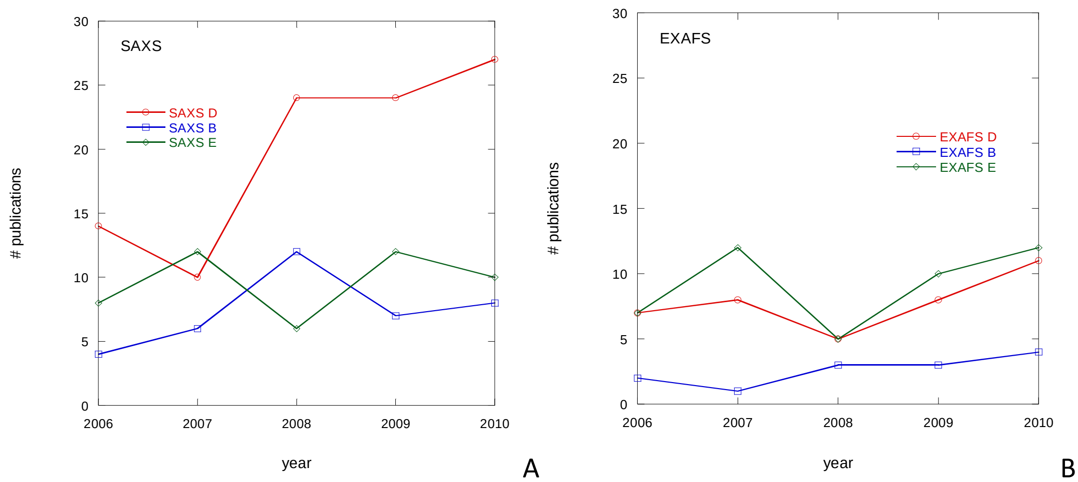

Figure 9.10
Publication output over the different techniques for Dutch (D), Flemish (B) and European (E) users.

On the SAXS station the ratio between the different user communities is as can be expected from the amount of beam time that each community is entitled to. On the EXAFS station this situation is slightly different. The European users appear to be more economical with their beam time. However, two remarks have to be made here. In the first place is the somewhat low Flemish output also a sign of the fact that this community is still in a development stage. Before DUBBLE there was hardly any XAFS carried out by Flemish groups. In the second place tend the Dutch users to engage themselves in more difficult on-line experiments with technique combinations. This results in a lower publication output but with papers in more prestigious journals.

When comparing with the European part of the beamtime one should also keep in mind that this part is supposed to represent the best of European research as perceived by the ESRF referees.

10 The international context

In order to make a relevant comparison with respect to the output and performance of DUBBLE in the international context it should be kept in mind that for different experimental techniques there is a different average amount of beamtime required to obtain publishable results. The Dutch users of the macromolecular crystallography beamlines require on average 2.6 shifts per publication. Techniques like Mössbauer spectroscopy and inelastic scattering, however, require about two weeks. Another factor that should be kept in mind is the number of beamlines and the ratio scientific support staff/beamline. More scientific staff in general means that more ‘aftercare’ in the form of help with data analysis and preparation for new experiments can be given to user groups by the beam line staff.

The comparisons that are made in this section are with established beam lines which have passed the stage of teething problems and can be deemed to be in ‘steady state operation’. The comparison is also made with the average of at least three recent operation years. It also can be remarked that the ESRF is at the moment the most productive operational synchrotron radiation source. A simple comparison with the publication numbers generated by the comparable Advanced Photon Source (Argonne, Illinois) will confirm this[6].

10.1 Comparisons per technique

10.1.1 XAFS

The DUBBLE XAFS beamline BM26A is fairly unique in the amount of catalysis research (>75%) that is carried out and in this respect there does not exist any directly comparable beam line. The on-line catalysis experiments are more complicated to carry out compared to experiments requiring a simple cryostat as sample environment. If we concentrate on the technique then the French ESRF FAME CRG BM30B[7] and the ESRF public beamline BM29 are comparable with the remark that >50% of the work on BM30B is carried out with either a simple cryostat or at ambient pressure/temperature.

	BM30B	BM29	DUBBLE/BM26A
5 year averaged # publications/year	25	31	20
Number scientific support staff	4	4.5	2
5 year averaged impact factor (based upon >100 publications)	3.73	not available	5.64

[6] https://beam.aps.anl.gov/pls/apsweb/pub_v2_0009.publication_stats_detail
[7] Based upon 2010 activity report, available via ESRF website

We can conclude that there is a relative low number of publications on this station but that the quality of the publications, as measured by average impact factor, is rather high. One reason for the relative low output is that the Flemish XAFS community is still rather new in the field and the output has not reached the state level that the Dutch community already has. The XAFS schools organized in the last two years in collaboration between Gent University and DUBBLE should have a positive effect on this.

10.1.2 SAXS

The DUBBLE SAXS beamline BM26B covers a large portfolio of subjects. However, experiments in the field of polymers are dominant and area major contributing factor to the forefront position that the ESRF has in this field[8]. Directly technique dedicated comparable beamlines in the steady state operation mode are rare at present. There are beamlines in the early phases of operation or under construction in Hamburg and Diamond and a larger number of beamlines on which SAXS/WAXS is only one of the techniques. The best comparison that can be made at the moment is with the ESRF ID02 public beamline, the APS Biocat beamline and the APS DND CAT beamline. This obviously with the caveat that for the Biocat beamline the subject of research is limited to biological specimens and that the DND CAT is specialized in polymers and has an elevated level of proprietary research which will not be published in the open literature.

	ID02 (ESRF)	Biocat (APS)	DND (APS)	DUBBLE/BM26B
5 year averaged # publications/year	46	27	28	37
Number scientific support staff	3.5 (+2 postdocs)	6	3	1 (+postdoc)

Here it can be remarked that the average of publication numbers for this station over the last three years is 43±2. The average publication impact factor for BM26B is 4.12. This is not known for the other beamlines.

10.1.3 Interface Diffraction

At present there are not many full time Interface diffraction beam lines operational. Within the last 3 years there has only been one successful proposal on BM26B and the last publication dates from 2007. There are two Dutch user groups that use the ESRF undulator beam line ID03. The group of Joost Frenken (Leiden) collaborates extensively with the ID03 researchers and has based PhD students on ID03.

This technique often requires extensive vacuum chamber preparation before an experiment can start. The ID03 beamline has two experimental hutches which allows one experiment to be built up whilst the other one is taking data thus minimizing the dead time between experiments. The beamline has 4 persons involved in user support and over the last years has a remarkable constant output of 20 ±1 publication/year.

[8] Thed N. van Leeuwen, Centre for Science and Technology Studies, Leiden ‘To which extent do Dutch scientists contribute to the output and impact of large research facilities?’

10.2 Comparisons per project

DUBBLE operates two beamlines simultaneously. As a project this makes it comparable with several APS CAT's as well as to the Swiss-Norwegian and Spanish Spline CRG operating at the ESRF. At the APS several CAT's have in the last years been taken over by the APS and are being converted from multipurpose beamlines to single technique beamlines in order to achieve the operational efficiency which is common at the ESRF. Therefore only comparisons with ESRF projects are made.

	techniques	#staff	#publications
Swiss-Norwegian	Single crystal HR powder diffraction Protein Crystallography XAFS	7 scientific support 1 technical 1 administrative	111
Spline	Single crystal HR powder diffraction Interface diffraction XAFS	5 scientific support 3 technical 1 administrative	26
DUBBLE	XAFS SAXS/WAXS Interface diffraction	4 scientific support 3 technical 0.2 administrative	75

The powder diffractometer is responsible for a large percentage of the SN output[9]. The protein crystallography is diminishing in importance since users prefer to use either ESRF undulator stations or the Swiss Light Source. The management of the SN project is convinced that their very high output rate is also related to the number of scientific support staff whom are (time wise) capable of providing aftercare, i.e. help with data analysis, for their users.

The budgets for DUBBLE and the SN CRG are comparable. Numbers for the Spline budget are unknown.

Regarding the support staff numbers one should keep in mind that the division of administrative tasks between the research councils and the CRG is not the same for every CRG.

10. 3 Comparison with ESRF beamlines

The ESRF, including the CRG's, has operated on average 44 beam lines in the last 5 years. Of these 8 are dedicated to macromolecular crystallography. The latter is a technique which is known to render a disproportional high number of publications which are also published in higher impact journals. Around 35% of the ESRF output is generated by these beamlines.

The 36 other beamlines cover a large range of subjects ranging from soft condensed matter to solid state physics and engineering. These beamlines produce at present annually about 1050 publications which renders an average output of around 30 publications/year/beamline. For DUBBLE this number, exclusive PhD theses is around 37.

[9] The ESRF ID31 beamline which is specialised in powder diffraction generates about 65 publications/year, i.e. twice the ESRF average. Also http://www.esrf.fr/UsersAndScience/Experiments/CRG/BM01/Publications/report/SNBL%20report%2010.pdf

To place this in perspective the reader is reminded that multi-year averages are used. The estimated confidence level for all these numbers is around 95%.

11 Future developments

The philosophy followed in the last 10 years with respect to developments has been to carry these out gradually in order not to disturb the user program and to remain within the allocated budget. The main developments have been in the implementation and development of sample environments and technique combinations. Also work has been done to extend the existing techniques with options which form a logical addition to the already existing infrastructure. The introduction of the electron yield EXAFS and the GISAXS are examples of this.

In principle there is no reason why DUBBLE should remain operating the same portfolio of techniques as at present. The original intention was to operate four techniques (SAXS/WAXS, XAFS, HRPD and ID). Already during the construction phase it was decided that HRPD would be exchanged for PX. Technical developments on the public macromolecular beam lines, i.e. the wide scale introduction from CCD detectors which increased the productivity of these stations by several factors, decreased the demand for beam time so much that the public beam lines could handle the Benesync BAG demands. Moreover the large size of molecules and small crystallite size studied by the Dutch-Flemish users require undulator beamlines since no bending magnet beam line can render the required low divergence. Therefore it was decided that the PX activities on DUBBLE would be terminated. No attempt has so far been made to set up a Belgian ESRF BAG although this would be quite beneficial for the Benesync ESRF juste retour numbers. The requirement for HRPD is rather low and is at present adequately covered by the exchange agreement with the Swiss-Norwegian beam line. For Interface Diffraction it was earlier recommended and decided that existing Dutch-Flemish users whom are self supporting can make use of the facility but that the DUBBLE staffing is too low to be able to support this scientifically nor that a large amount of technical support can be made available.

In order to asses if it would be worthwhile to consider additional techniques one has to solve a complex equation which includes the technical feasibility, the impact this will have on the existing program, the financial applications and the potential user demand. For the latter one also has to take into consideration if this demand can, or cannot, be satisfied by access to the public ESRF beamlines or in collaboration with other SR sources.

11.1 Inventory of Dutch-Belgian SR use

An exhaustive review of which X-ray based techniques would require sufficient beam time and number of user groups to make it worthwhile considering to implement on DUBBLE is beyond the resources and time scale for this review. For instance this should encompass research into potential demands by user groups not part of the established user synchrotron laboratory community.

Dr. Martin Feiters, Dutch representative with the European Synchrotron User Organization (ESUO) has obtained an inventory of Dutch institutes active in European Synchrotron Facilities.

Unfortunately the ESUO data base only shows which institutes are active, not which group, nor what station/technique has been used or which volume of beam time. However, it is clear that besides the ESRF the most used facilities are BESSY, SLS and DESY. The first two institutes offer more specialised beam lines. Bessy in the soft X-ray range, which is not available at the ESRF, and the SLS in for instance a coherent SAXS line and a specialization in microfocus spectroscopy lines as well as soft X-ray beam lines. A non-comprehensive investigation of the publication data bases, as well as enquiries with staff members from three main laboratories[10] shows that the bulk of SR based publications for Dutch-Belgian users (80±5%) is being generated at the ESRF. Of this number 45% of the total and over 50% of materials science publications is generated on DUBBLE.

Non-European sources are being used by Dutch-Flemish users as well. However, this is somewhat limited. Not necessarily due to travel distances but also due to the restrictive policy from the USA with respect to visa for non-Europeans. Some use of the ALS, APS, Taiwan and Spring8 is known but this is based mainly on personnel contacts or highly specialized beam lines not available on European sources. Wallonian users are known to be using Soleil but we have not been able to obtain figures for this[11].

An analysis can be made of the output generated by Dutch-Belgian users on the public ESRF beamlines. For this the ESRF database 2004-2009 has been consulted. See appendix 4. This database is not complete since the output of DUBBLE, as known to the project leader, is about 20% higher than what is known in the database. Without making a claim to completeness we can make an analysis and assume that the omissions in the ESRF database are statistically distributed and not specific to any research area or beamline.

For the most utilized techniques the total ESRF and DUBBLE output is shown in figure 9.8. This analysis shows that for the techniques that DUBBLE offers, either directly or via collaborations with the Swiss-Norwegian CRG, the user community is also rather successful in obtaining beam time on the public beamlines in the open competition. In fact to the level that the 6% of beamtime that Benesync users are ‘entitled’ to on the public ESRF beam lines are fully used.

The large fraction of publications on High Energy Diffraction are related to beamline ID11. This is a general purpose line with a wide energy range and part of these experiments could have been carried out on several other beamlines as well. There is only few Dutch-Belgian users that utilise the energy range > 60 keV, which is the real specialty of this line. The number of publication in Interface Diffraction is due to only two groups. A slowing down in the activity of any of these groups, like what has happened over the last three years, has a profound effect on the output rate.

The high output of the Benesync MX community is not associated with a high demand in beamtime[12]. On average the user group required only 2.6 shifts/publication (ESRF average 4 shifts/publication) and has received 4.6% of the beam time on the available beamlines. However, the Benesync output in this field represents 7% of the total ESRF MX output. Around 10% of the beamtime offered to the

[10] SLS, Prof Friso van der Veen; Diamond, Prof Nick Terrill; Hamburg, Dr. Sergio Funari
[11] For the ESRF the Flemish useage is substantially higher compared to the Wallonian.
[12] Information on MX use obtained from Dr. Sean McSweeney (head ESRF MX group) and Dr. Peter Zwart (ALS)

users is not taken up. The amount of MX beam time available worldwide and the efficiency of the beamlines is predicted to increase in the coming years[13].

11.2 FEL's and table top synchrotrons

The introduction of X-ray free electron lasers will open up new vistas for research. However, to use the terminology 4th generation synchrotron radiation sources for these machines is somewhat misleading. In the first place the number of beamlines that can be operated with these facilities is much smaller compared to SR sources. The pulsed peak intensity of FEL's is indeed much higher than what one can expect from a conventional SR source. When considering the time-averaged flux it is clear that SR sources are better. For the average materials science experiment where one wants to follow the evolution of a sample in time or as function of photon energy the SR sources will remain as important as before and a prolonged exposure to the very high peak intensity will be a threat for the sample integrity. FEL's and SR sources should be seen as being complementary and not as competitive.

The main 'threat' to the large scale SR facilities will become the 'table top' SR sources, that could drive 2-3 beamlines, that are presently under development. However, before this is technically sufficiently developed and commercialised to be interesting for university departments to obtain will be a matter of many years (estimated 5-10).

At the Reactor Institute Delft a new SANS beamline will be installed in the coming years. In combination with a new cold source this could become an instrument that provides information in the same size regime as the DUBBLE SAXS beamline. However, the instrument will not be suitable for time-resolved experiments and will not be able to handle the volume of user groups that DUBBLE can. In fact it is a very exciting development that Dutch researchers will be able to benefit from the complementarity between the two techniques.

11.3 Demand for other techniques or instrumentation development

At present one can distinguish several trends which have been made feasible by technological devlopments. The increase in the use of coherence in the beam for diffraction and imaging is clear. However, the coherent fraction of an ESRF bending magnet is low compared to the undulators and also lower compared to more modern sources. Experiments are feasible and have been done on BM26B (and BM02) but these are time consuming due to the low coherent countrates. It should be noted that the ESRF upgrade will not result in an increase in the beam coherence.

There is also a clear trend in implementing microfocus optics (e.g. ESRF upgrade program). DUBBLE has already implemented such optics on both beam lines and with still acceptable flux. Spot sizes of around 10 microns are achievable. However, a further reduction to submicron levels is not realistic with the characteristics of the bending magnet source at the ESRF (collimation less compared to ESRF undulators).

The different forms of imaging/tomography are gaining importance at present. This is partially due to improved X-ray technology but also due to improved computing capabilities. For some forms of imaging it might be possible to be implemented on DUBBLE. In fact, work on BM26A has already

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[13] Several new beamlines at Diamond and Petra 3 will become active in the coming years.

generated the first element specific tomographic results[14]. This development was set in motion to establish if it was also feasible to perform confocal XAFS experiments simultaneously with the imaging. However, it should be kept in mind that not all types of imaging are feasible and that for some techniques this might require expensive and time consuming adaptation of the optics.

A possible case can be made to implement biological solution scattering on the SAXS beamline. This technique is growing in demand to provide complementary data to macromolecular crystallography. Expereince has shown that, although feasible, this technique is most efficiently performed on a dedicated beamline with sample handling robots. One of these beamlines has been constructed at the ESRF (with help and expertise from DUBBLE staff). Another such instrument is available at the EMBL in Hamburg. With the number of interested user groups in Netherlands-Flanders being limited to around 8 and the amount of beamtime/session estimated to be 1-2 shifts on a fully automated beam line it does not appear to be logical to make a major investment in this field.

11.4 Conclusions

From the numbers available at present there is no clear demand for a specific new technique by the existing SR user community although for some techniques an increase in the available beam time would be welcome. Some beam time is required on highly specialized beamlines but this is in general from individual groups and often on a 'one-off' basis.

However, this could be misleading. From research into the use of SR sources by the American Institute of Physics one knows that the average beam line oversubscription rate stabilizes at a factor of 150-200%. Too high an oversubscription with a too small probability to obtain beam time ensures that supervisors steer PhD research into different directions which might be 'sub-optimal' from a research perspective but at least guarantee sufficient results for PhD students to graduate..

For the techniques available on DUBBLE the user community is also using equivalent public ESRF beam lines with a success rate in the open competition which is comparable or higher than the ESRF average.

A broad and deep overview of the existing and potential requirements is beyond the resources available to DUBBLE staff and should be carried out by the research councils.

12 SWOT analysis

The issues that are being addressed in this section are answers to questions suggested by the NWO team responsible for the organization of this review and might overlap to some degree with previous chapters.

The strengths of the DUBBLE project

- The limited size and stability of the user community allows investment in experimental infrastructure tailored for this Dutch-Flemish user community. This is in contrast to

[14] Group L. Vincze (Gent) in collaboration with DUBBLE staff

comparable ESRF beamlines which have to satisfy a much larger and more fluctuating user group.

- Worldwide there is a shortage of XAFS and SAXS/WAXS beamlines. Due to the rather large dependence of the Dutch and Flemish economy on food and chemical industries and the increasing importance from nanotechnology in general these are techniques that are in high demand from many groups within Belgium and the Netherlands associated with the academic research relevant for these industries. DUBBLE is well poised to address this demand.
- The existing infrastructure allows for the rapid interfacing of complicated sample environments and additional experimental techniques which makes experiments feasible which cannot be carried out anywhere else unless with great difficulty. The qualitatively very high level catalysis experiments are a good example of this as well as the pioneering role in the introduction in pulsed high magnetic fields.
- The pioneering role in technique combinations that the NWO beamlines traditionally have had attracts international high level researchers. The cross fertilization that can occur when these groups start collaborations with Dutch or Flemish groups is beneficial for the national research landscape.
- The very limited number of Dutch and Belgian scientific staff in the ESRF central laboratory is one of the reasons that the ESRF is underused. DUBBLE guarantees at least a certain form of national presence at the ESRF which can also act as an antenna for ESRF developments for the funding agencies.
- Internationally the DUBBLE beamlines have a very good reputation for reliability, data quality and the sophistication level of the experiments.
- The publication output of DUBBLE is both quantitatively as well as qualitatively high. Knowledgeable SR laboratory directors like H. Padmore (ALS) and F. van der Veen (SLS) have classified it as ‘outstanding’.
- In the first ten years DUBBLE has not been plagued by budget problems. This has enabled the development of very reliable and cost effective beam lines and at times made it possible to find alternatives solutions to problems due to manpower shortage.
- A large fraction of the Dutch and European user groups are internationally recognized. The Flemish user community is newer with respect to the use of SR but is growing in quality.
- Both beamlines have been upgraded in the period 2007-2010 to a level that will allow a high level of experiments for the coming 7 – 10 year. Both SAXS/WAXS as well as XAFS are very well matched to the ESRF bending magnet spectrum.

The weaknesses of the DUBBLE project

- The small amount of user support staff does not allow a high level of ‘user aftercare’ for a broad user group and only limited time for training. This sometimes results in collected data sets not being used since users lack the experience to handle these themselves. In time, with user groups gaining more experience, this problem is slowly reducing but at times it proves a barrier for new groups.
- The fact that DUBBLE is not embedded in a ‘home institute’ has as a consequence that it is difficult to find and retain staff. There are no promotion possibilities and it is more difficult to

set up larger scale collaborations and have access to sample preparation facilities. The latter is an obstacle for the in-house research of younger (non-permanent) staff.

- Both beamlines are used heavily and successfully for the two major techniques SAXS/WAXS and XAFS. Interface Diffraction has hardly been used in the period 2007-2011 (although the diffractometer itself might play a role in newly developed GISAXS experiments). A rejuvenation of this technique will be at the expense of the SAXS user program and it is doubtful if this is useful in the light of the availability of ID on other ESRF beamlines. It will also require additional staff with sufficient expertise in this field. (This in addition to the extra staff that will be required to operate the two main techniques)
- Most of the expertise within DUBBLE on the operation of the beamlines, the research landscape suitable for the DUBBLE beamlines and insight in the feasibility for further development is vested in two persons. One of these, after 10 years service, still does not have a permanent position. This is a very fragile basis.

Opportunities

- The development philosophy so far has been one of gradual improvements to the optical systems, sample environments and experimental infrastructure. In the light of the output we consider this to be a success. There are opportunities in continuing with this policy but also it can be contemplated to investigate if there would be a large demand for new techniques suitable to be implemented on an ESRF bending magnet. This would require a thorough investigation from the national research landscape with advice from international experts.
- Not all potential user communities have been reached yet. Biophysics, ceramics, cultural heritage are among the areas where there are opportunities for enlarging the user community. With extra manpower this issue could be addressed. However, one should keep in mind that for a successful user program a regular access to the facilities is required and that the amount of available beamtime is intrinsically limited.
- There are still large opportunities in the further expansion of the available sample environments. Especially with the recently introduced microfocus options one can think of the further development of microreactors, stop-flow experiments, facilities for inhomogeneous samples etc. This is in line with the wishes of the present user group but can also attract new user groups from a wide variety of fields.

Threats

- There are several SAXS/WAXS and XAFS beamlines worldwide available. However, only at the ESRF public beamlines Dutch and Flemish users are entitled to beamtime. For all the other sources the beamtime will be limited or only via collaborations with other groups. This cannot render the volume of beamtime that is required at present. Alternative radiation are not suitable (XFEL) or still in the distant future (table top synchrotrons). There is at present no threat that there will be a shortage of users.
- Organizational there are several threats in the governance structure that can only be addressed by the research councils.
- The internally fragmented funding sources within NWO are worrying.
- The financial situation in the last years has been satisfactory apart from the fact that there is too little budget for extra staff available. This poses a threat to initially the user service but

- ultimately to the durability of the project. Also it can be foreseen that budget adjustments for inflation, which have not been made in 10 years, should be implemented.
- The changes within the ESRF, due to the 'Upgrade Program' do not pose a direct threat apart from some local issues regarding space and accommodation. With effective action from the representative bodies of the research councils towards the ESRF management this can be sorted out.

Strategy for the next period

At present DUBBLE is well placed to serve the demands of the existing user group and can provide excellent data quality and, when compared internationally, at a very high level of experimental sophistication. The output of the beamlines is also at a very high level and still increasing. Since around 50% of the Dutch-Belgian SR based material science publications are being generated at the DUBBLE beamlines one can conclude that nationally the existence of DUBBLE is quite relevant.

The strategy for the coming years:

- Keep gradually improving the infrastructure with respect to microfocus, detectors, beam stability without endangering the existing user program.
- Sample environments are the strong point of many of the successful user projects. We should keep investing and continue developing these.
- Stimulate data analysis workshops in order to improve the expertise in the existing user community. Further develop data analysis methods in collaboration with other SR laboratories.
- Try gradually to bring in new user groups and provide sufficient support to initiate and train these users in the use of the experimental techniques by either collaborations with staff members or to arrange that these groups are being supported by existing groups via collaborative projects.
- Try to interest researchers from areas so far not or hardly present at DUBBLE. Growth area here could be for instance biophysics.

With regard to the desirability of the introduction of new techniques on DUBBLE this is not a decision that could or should be taken at the level of DUBBLE. DUBBLE is part of the wider Dutch-Flemish X-ray infrastructure. At the national level an inventory should be made what is present and what is required. This not only with the existing user community in mind but also in the perspective of international developments and interests of user groups traditionally not using SR. This is too broad a task for the DUBBLE staff on its own and should be organized by the policy departments of the research councils.

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Our colleagues Wim Bouwman, Martin Feiters, Han Goossens, Bart Goderis, Guy Luijckx are thanked for providing information and advice. Colleagues from other SR facilities Friso van der Veen (SLS), Peter Zwart, Howard Padmore (ALS), Sergio Funari (Hasylab), Nick Terrill, Trevor Rayment (Diamond) are acknowledged for their help and information. Sophie Rio from the ESRF library has provided the data on publications and Joanne McCarthy was very helpful in providing the beam time statistics.

Agnes van den Broek (NWO) has provided the financial oversights and Murielle Rigolet (ESRF CRG office) has gathered the ESRF financial data. Francien Petiet, Mirjam Rigterink and Leontien Hullemans have been very helpful. Obviously the DUBBLE team has helped in a great way with this report.

This report is written by the project leader W. Bras whom was assisted by the adjunct project leader G. Luijckx. However, W. Bras is responsible for any errors in the content.

Appendix 1 Beamlines technical

The optical system of the beamlines has not fundamentally changed since the previous reviews. Beam position monitors and feedback loops from these monitors have been installed or are going to be installed in the ESRF upgrade shutdown. This improves the beam stability and beamline reliability but is less relevant for the overall picture. In this section only a very brief description of the optics is given.

Bending magnet BM26 is the radiation source for the DUBBLE beamlines. As usual at the ESRF this magnet doesn't have a uniform field but has a 0.4 Tesla and 0.8 Tesla section. BM26A uses the 0.4 T radiation and BM26B the 0.8 T. There are marginal differences. Both beamlines receive significant flux in the 4 – 60 keV photon energy range.

The experimental hutch wall thickness of BM26A is cleared for white beam operation, i.e. also suitable for higher energies. However, extending the range from BM26A to higher energies would require extra Brems-strahlung shielding and photon shutters. BM26B is limited to 30 keV photons.

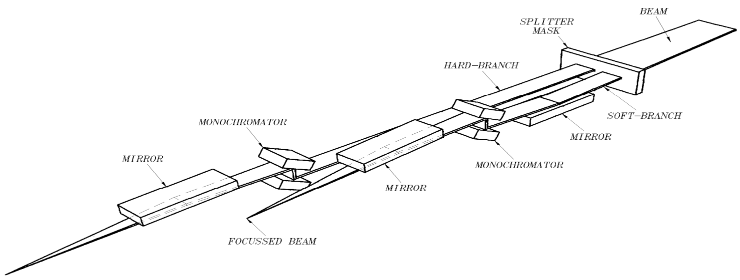

Figure A1
The schematic optical lay-out from the beamlines. BM26A (soft branch) and BM26B (hard branch)

The collimating mirror on the soft branch will be installed early 2012. On both beamlines the focusing mirrors and monochromators are installed.

	BM26A	BM26B	unit
Energy range	4 – 42	5 -30	keV
Maximum Flux	> 10^{12}	> 10^{12}	ph/sec
Spot size			
Normal	0.3 x 1	0.3 x 0.3	mm^2
Microfocus 1	8	12 (KB system)	μm^2
Microfocus 2	-	10 (CRL)	μm^2
ΔE/E	1.8 x 10^{-4} (with collimating mirror)	2.4 x 10^{-4}	

Appendix 2 User groups

In this appendix the names are indicated from research group leaders with independent research lines. There is a large amount of cross collaborations between groups and accros techniques and often the personnel for the beam time is pooled between groups. There are also part time appointments spread over different universities. Therefore it is nearly impossible to disentangle all information. In the Dutch and Flemish section new user groups compared to the 2007 review are indicated in Italics.

Dutch Universities

Groningen

- G. ten Brinke/K. Loos

Twente

- D. Blank
    - *A. ten Elshof*
    - S. Harkema

Amsterdam

- *G. Rothenberg/H. Castricum*
- G. Wegdam

Delft

- *W. Bouwman*
- *E. Kelder*
- *E. Offerman*
- *R. Kapteijn*
- *J. Dik*
- *H. Terryn (also Brussel)*
- *R. van der Krol*

Utrecht

- Weckhuijsen/de Groot
- H.Lekkerkerker/G.J. Vroege/A Pethukov
- *T. Behrendts*
- A van Blaaderen
- *M. Wolthers*

Eindhoven

- H.E.H. Meijer/G. Peters
- E.W. Meijer
- P.Lemstra/H. Goossens
- *D. Broer*
- A. Schenning
- C. Koning
- E. Hensen/R. van Santen
- *T. Peys*

- *R. Sybesma*
- E. Nies (also Leuven)

Wageningen

- M. Cohen Stuart
- *P.N. Lens*

Leiden

- J. Bouwstra

Nijmegen

- M. Feiters
- E. Vlieg

Dutch Research Institutes

ECN Petten

W. Haije

Nizo

R.H. Tromp/ C. de Kruijf

Amolf

G. Koenderink

Astron (Utrecht)

E. Costantini/C. de Vries

Flemish user groups

K.U.Leuven

- B. Goderis
- K. Temst/A. Vantomme
- *P. Lievens/M. Van Bael*
- C. Kirschhock
- *B. Sels*
- *P. Van Puyvelde*
- *G. Van Den Mooter*
- *K. Binnemans*
- *J. Delcour*
- *R. Swennen*
- *J. Elsen*
- A. Maes
- E. Nies (also Eindhoven)

Ghent University

- *R. Van Deun*
- K. Dewettinck
- *P. VanderVoort*
- A. Adriaens
- *F. Duprez*
- D. Poelman
- *L. Vincze*

Hasselt University

- M. Van Bael

Vrije Universiteit Brussel

- B. Van Mele/G. Van Assche

- H. Terryn (Also Delft University)

Flemish Research Institutes

Belgian Nuclear Research Center - SCK-CEN , Mol

- N. Maes

- M. Honty

Institute for Agriculture and Fisheries Research, Merelbeke

- K. Smet

International User groups

Acces to the DUBBLE beamlines in the general user time is arranged via the ESRF administration. In this section only the most recurring groups are mentioned. Also indicated is the existence of major collaborations with Dutch/Flemish groups.

Israel

U. Raviv/C.R. Safinya (St Barbara US)

R. Shenhar

Y. Golan/J. Israelachvili (St Barbara US)

United Kingdom

R.C.A. Catlow (UCL, also via Utrecht)

A.J. Ryan (Sheffield)

F. Volrath (Oxford, also via Eindhoven and AMOLF)

I. Hamley (Reading)

M. Tromp/J. Evans (Southampton)

T. Rayment (Diamond, also via Brussel)

Ireland

M. Ryan (Dublin)

France/Wallonie

D. Ivanov/G. Hadziannou (Mulhouse, also via Leuven)

C. Gommes (Liege, also via Leuven)

A. Khodakov (Lille)

Switzerland

P.Smith/T. Tervoort (ETH Zurich, also via Eindhoven)

R. Daehn (Paul Scherrer Institute)

J. van Bokhoven/R. Prins (ETH Zurich)

United States

J. Kornfield (Caltech, also via Eindhoven)

Italy

C. Lamberti (Torino, also via Utrecht)

G. Alfonso (Genua, also via Eindhoven)

Norway

O. Fossum

D. Nicholson (Trondheim)

Appendix 3 Industrial relevance of DUBBLE

The group of Prof. Joke Bouwstra (Simon Stevin meester 2005) has received over 3.5 M€ to perfrom studies on the structure of skin and eczema. For five PhD students funded by either STW or industrial funds crucial parts of their thesis depended on data collected at the DUBBLE beamlines and patents have been obtained. Industrial partners that can be named are Unilever, River Diagnostics and Leo-Pharma (Denemark).

The group of H.E.H. Meijer/ G.Peters has received STW and DPI funding for 7 postdocs/PhD whose work hinged on DUBBLE data. Projects ranged from flow induced polymer crystallisation to materials behaviour under mechanical deformations. Major industrial partners in these projects included BASF, Borealis, Braskem, Dow Benelux, DSM, Exxon Mobil, LyondellBasell, Sabic Europe, Sabic Innovative Plastics, Teijin Wavin Technology & Innovation, Moldflow (*Victoria, Australië),* Kiwa Gas Technology, Intertek Polychemlab (Geleen, The Netherlands), IME Technologies, Purac Biochem

In the group of B. Weckhuysen (Utrecht) around 40% of the postdocs/PhD positions is funded private-public or private. The private-public funding route consists of M2i, ACTS en CatchBio initiatives whilst the industrial partners, interested in processing catalyst include Shell, ExxonMobil, Dow Chemicals, BASF, SK Energy, Albemarle Catalysts, Total, Sumitomo and Rhodia. Besides this there are companies specialized in biomass conversion like Avantium en Croda and the automotive industries like BASF, DAF en Toyota. A crucial part of the research here depends on the unique possibilities at DUBBLE to combine different techniques on-line. Around 10 students of this group have collected important parts of their thesis on DUBBLE.

The group of Kelder (Delft) has been instrumental to obtain funding for a postdoc to be placed at DUBBLE via the European private-public Alistor network (http://www.alistore.eu). The main activity will be the development of Li-ion battery for traction purposes. Industrial partners include Volvo, Renault and Spijkstaal (car manufacturers) and GAIA AkkumulatorenWerke (battery manufacturer).

The Energy Centre Netherlands (ECN) has used DUBBLE in the framework of an EU FP7 project in which Air Products and BP are major industrial partners for applications and process scale-up.

Several other groups have also acknowledged industrial funding for DUBBLE related research. Companies involved in this are among else Tata Steel Europe, Ocas - Arcelor Mittal, SKF, Nedschroef, Ovako wire, Kodak, OCE, Jansen Pharmaceuticals, Loreal.

Appendix 4 Benesync use of the ESRF

The useage of the ESRF by the Benesync consortium is already for many years below the 'juste retour' level to which one is entitled based upon the contribution to the ESRF budget (5.8 %). In figure A4.1 the development of the application pressure and allocated shift percentage is given. In the 'juste retour' calculations 25% of the Dutch-Flemish beamtime on DUBBLE is counted as part of the ESRF 'juste retour'. DUBBLE contributes 2 x 0.35 = 0.7% on top of the numbers shown here. The target for Benesync is a juste retour of 5.8 %.

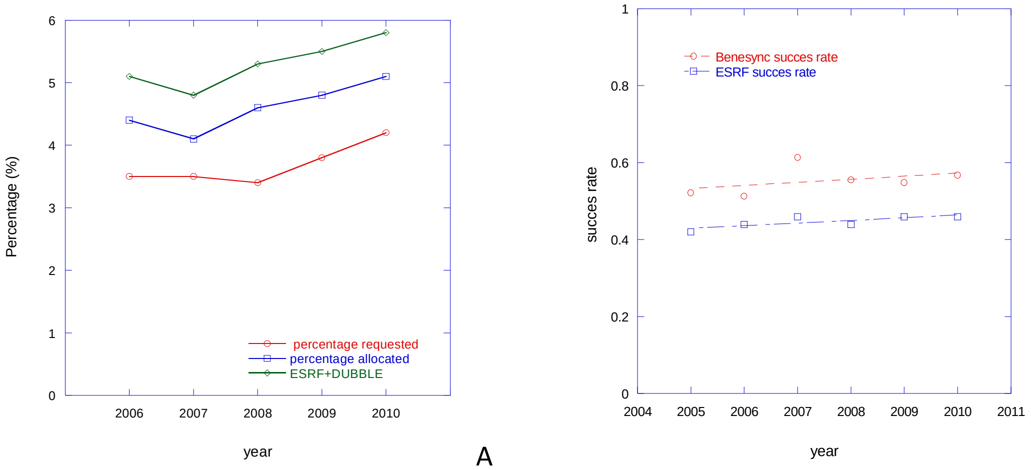

Figure A4.1
Panel A Application pressure and allocated shifts on public beamlines ESRF beam lines for the Benesync consortium in percentages. Panel B Success rate for Benesync proposals compared to average ESRF success rate.

These figures indicate that when Benesync users apply for beam time they are in general more successful than the ESRF average but that one simply does not apply for sufficient time on the public beam lines.

An interesting parameter as well is the success rate as function of research area. See figureA4.2

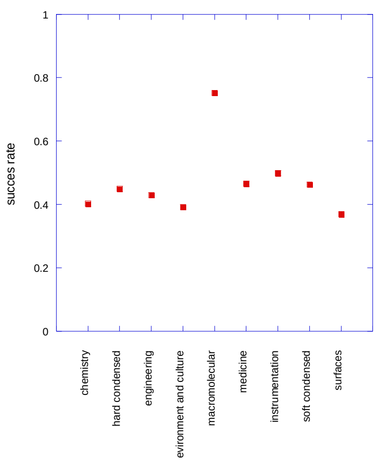

Figure A4.2

Benesync application success rate on ESRF public beamlines as function of research area time averaged over period 2006-2010.

The high success rate for the category Macromolecular Crystallography is probably due to two factors. In the first place the high level of the applications. In the second place it is indicative of a lower oversubscription rate for these beam lines.

The ultimate goal when using central facilities is obviously not the success rate in obtaining beamtime but the success rate in publishing the data. An easy accessible parameter is the number of publications.

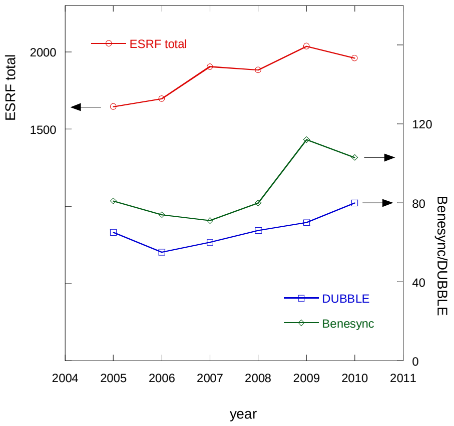

Figure A4.3

The total number of ESRF publications (left scale) and Benesync and DUBBLE publications (right scale)

In figure A4.4 the number of Benesync publications on public beam lines as percentage of the total number of ESRF publications is given. Also the juste retour percentage of beam time is plotted. The total number of manuscripts, i.e. including DUBBLE, with at least one Dutch or Belgian co-author is shown.

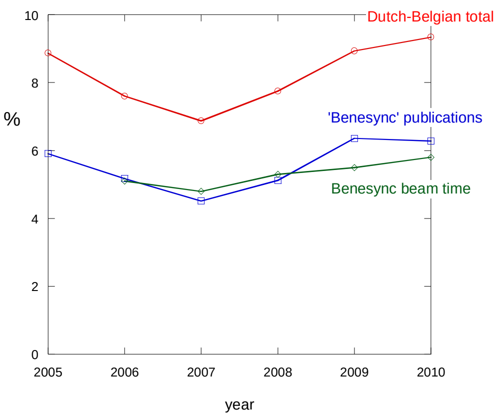

Figure A4.4

The percentage of Benesync manuscripts, the percentage of 'juste retour' beam time and the total 'Dutch-Belgian' output of the ESRF.

One is reminded that the Benesync 'juste retour' percentage of beam time also includes 25% of the DUBBLE beamtime. In order to make a reasonable comparison the pure number of manuscripts from the public beamlines is adjusted with 25% of the DUBBLE output as well.

For the research councils it might be interesting to not only compare the bare numbers but also take into account the quality of the journals in which the manuscripts have appeared and possibly the subdivision in Dutch and Belgian numbers. This, however, would require a major effort and is of less relevance for the review of the DUBBLE project.

Note: It can be mentioned here that the number of staff of Dutch and Belgian origin in scientific functions at the ESRF is very limited and far below the 6% level that it should be according to the financial contributions from Benesync. This results in an, compared to other countries, underdeveloped social network between researchers in Belgium and the Netherlands and ESRF scientist. Via these networks often new research is initiated. It would be very useful to investigate how this situation can be improved.

Data regarding the 'juste retour' and application pressure numbers was provided by Joanne McCarthy (ESRF user office). Bibliographic data by Sophie Rio (ESRF library).

Appendix 5 Publications Dutch and Belgian users per ESRF beam line

Publications with at least one Dutch or Belgian author over a 5 year period. These data are derived from the ESRF publications data base. No claim to completeness is made. However, there is no reason to assume that there would be systematic errors in the distribution over the beam lines. Beamlines that will be closed due to the ESRF budget cuts or for other reasons are indicated in *italic*.

Beamline	#publications	Beamline technique
BM1	19	Swiss Norwegian CRG (exchange agreement)
BM5	2	
ID01	0	anomalous scattering
ID2	24	SAXS
ID3	12	Interface diffraction
ID8	11	soft X-ray spectroscopy
BM08	2	
ID09	*3*	*High pressure*
ID10B	11	Soft matter general purpose
ID11	33	High energy diffraction, general purpose
ID12	1	circular polarisation
ID13	4	micro focus diffraction
BM14	17	protein crystallography
ID14	71	protein crystallography (4 beam lines)
ID15A	8	High energy diffraction/scattering
ID15B	1	
BM16	*6*	*Spanish CRG*
ID16	2	inelastic scattering
ID17	3	Medical (also cultural heritage)
ID18	3	nuclear resonance/fluorescence
ID19	1	topography
ID20	*1*	*magnetic scattering*
BM20	1	ROBL CRG
ID21	2	fluorescence
ID22	2	nuclear resonance/fluorescence
ID23	18	protein crystallography (2 beam lines)
ID24	4	time resolved EXAFS
ID26	4	high resolution EXAFS, RIXS
BM26A	53	DUBBLE EXAFS
BM26B	110	DUBBLE SAXS
ID27	0	high pressure
ID28	0	inelastic scattering
BM28	4	multipurpose
BM29	7	EXAFS
BM30	1	EXAFS
ID29	11	protein crystallography
ID31	8	powder diffraction
ID32	*0*	*surfaces and interfaces*
	460	

Appendix 6 In-house research

Besides the beam line support duties all scientist working on the DUBBLE beamlines are also involved in in-house research. Part of this work is instrumentation research and part of this is wider ranging. Apart from W. Bras all scientists working at DUBBLE can be considered to be 'early career' researchers. There are many collaborative efforts with external user groups. Overall supervision is by W. Bras.

S. Nikitenko
Involved in the development of Beam Position Monitors and the development of methods to accommodate multiple technique combinations. Also involved in time-resolved studies on vitrification in glass ceramics (Dow Corning)

G. Portale
Develops the GISAXS methods further as well as the development of microfocus options.
The main research centers around membranes for fuel cells, metal containing micelles and polymer processing. Is also involved in the development of orientation methods via high magnetic fields (in collaboration with the Nijmegen High Magnetic Field Laboratory and A. Schenning)

M. Silveira
Develops confocal energy dispersive diffraction for the studies of cultural heritage artefacts.
Collaborates on projects on geochemistry and soil contamination using on-line XAFS and diffraction methods.

Postdocs

D. Hermida
DPI postdoc. Develops instrumentation for on-line supercritical CO_2 processing with the intention to utilize this for self assembly processes of core shell particles (Luik University, TUE and Nottingham). Is responsible for polymer deformation studies in collaboration with H. Goossens and templated crystallization in collaboration with N. Sommerdijk

Vacancy
Alistor postdoc. Develops the XAFS electron yield system for on-line electrochemistry. This will be applied to materials relevant for battery research.

V. Martis
Phd student (University College London)
Has developed the 'dry' electron yield system in order to be able to distinguish between bulk and surface catalytic activity of materials in a single experiment. To this effect he has also co-designed the

high pressure gas system to be used with the electron yield experiments. These systems have been used for Fischer Trop catalysts. (end date September 2011)

H. Islam
Phd student (University College London)
Will continue the work started by Vladimir Martis but the emphasis will shift towards different catalytic materials. These systems will be studied in a time-resolved mode.

W. Bras
Supervision of most of the research projects mentioned above.
Interested in:
- bio-polymers under external fields (shear, magnetic, tensile). Initiated a 4 way collaboration with F. Volrath (Oxford), G. Koenderink (Amolf) and H.E.H Meijer/G. Peters (Eindhoven).
- vitrification processes in glass ceramics (Dow Corning and G.N. Greaves)
- on-line catalysis and difference between bulk/surface catalysis (with C.R.A. Catlow, UCL)
- on-line polymer processing (strong collaboration with A.J. Ryan, Sheffield)
- use of on-line pulsed and static magnetic fields (also involved in the Euromagnet network, i.e. Nijmegen, Grenoble, Dresden and Toulouse)
There are several projects in which W. Bras is involved. Involved in 7-10 publications annually.

Appendix 7 Recommendations review committee 2007

The committee for the 2007 review gave 11 recommendations. These were not only aimed at DUBBLE but also at the participation of Benesync in the ESRF. For the complete text of the recommendations one is referred to the document on the accompanying disk. Here we will address the issues raised in 2007.

1. **NWO and FWO were advised to continue the DUBBLE project and participation in the ESRF.** This advice was followed.

2. **It was advised to investigate collaborations with other CRG's to make more techniques available.**
   The collaboration with the Swiss-Norwegian CRG has continued and has resulted in several powder diffraction and EXAFS/Raman publications. Attempts to establish a similar deal with the Spanish CRG for the exchange of ID beamtime has not been successful. Informally beam time has been exchanged with the ROBL CRG for work on radioactive samples

3. **The steering committee should play a more proactive role in the acquisition and training of new user groups and attempt to bring user groups to the public beamlines.**
   In the new governance structure this role was transferred from the steering committee to the program committee. In the period that the SC was still responsible there was no discernible activity in this area nor is there any formal activity from the PC at present.

Training of EXAFS users in data analysis was organized by collaboration between Gent University and DUBBLE. A similar initiative for SAXS is planned in 2011 (Delft, DUBBLE, Groningen).

The public beamlines that are providing similar techniques, although not the high level of infrastructure, as DUBBLE are already used to the full extent by Dutch and Flemish users who are already proving that they are able to get beamtime in open competition.

4. **The steering committee should play a more proactive role to obtain extra financing**
   In the present governance structure it is not clear who is responsible for this.

5. **The DUBBLE staff should hold 'intake' meetings with new user groups**
   To the experience of the local team this is hardly an issue anymore. However, this definitely should be heard from the user's side as well. Hopefully the questionnaire associated with this review will shine light on this.

6. **To increase the number of staff**
   The number of user support staff has not increased. There are no funding programs that allow to apply for user support staff and this has to be handled at a more structural level. The first opportunity is the renewal of the Flemish 'Big Science' grant.

7. **To improve the quality of the Human Resource Management by both NWO as well as FWO**
   In the period since 2007 two positions have been converted from temporary to permanent. The number of man-months that people have experienced with health insurance has been reduced but it has still happened that staff members were uninsured for extended periods. Problems about expatriate allowances have caused one staff member to seek employment elsewhere. The career perspective of the employees has not changed. The staff income levels are still structurally too low compared to the surrounding institutes and comparable projects in the Netherlands. Especially when one also takes into account the higher workload compared to the surrounding institutes. On the Flemish side there is still the situation that a staff member after >10 years with DUBBLE still doesn't have a permanent position.

8. **To put the funding from FWO on a more structural basis**
   -

9. **To ensure that a sufficient operation budget would be available**
   The budget has not changed and has been sufficient so far. However, after 10 years without inflation correction it should be realized that might lead to problems.

10. **For NWO and FWO to make sure that relevant information regarding the use of the public ESRF beamtime would be available.**
    This issue is less relevant in this review since the ESRF use is not under scrutiny. However, the projectleader DUBBLE has gathered some of this information which can be found throughout the report whenever it is relevant to asses DUBBLE and in appendix @.

11. **For NWO and FWO to make sure that the 6% ‘juste retour’ of the public ESRF beamtime would be achieved.**

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