Project No. FP7 – 212348

NFFA

Nanoscience Foundries and Fine Analysis

D4.8

Definition of Quality Standard for NFFA

Work Package	**No.4**
Work Package Title	**Development of management structure and format of user access for NFFA-RI Centres. Design of NFFA Data Repository and access criteria. Intellectual property issues.**
Activity Type	**RTD**
Lead Beneficiary	**No.1 CNR-IOM**
Estimated P/Ms	**6**
Nature	**Report/Prototype**
Dissemination level	**Public**
Delivery Date	**Contractual M 24 Actual June 2010**
Task Leader	**R. Gotter (CNR-IOM)**
Major Contributors	**D. Orani (CNR-IOM)**
Other Contributors	**R. Ciancio, C. Africh, G. Rossi (CNR-IOM), L. Fonseca (CSIC-CNM)**

Delivery Slip

	Partner/Activity	Date	Signature
From	CNR-IOM	28/06/2010	Gotter, Orani
Reviewed by	R. Ciancio, C. Africh, G. Rossi, R. Ferranti	30/06/2010	All
Consistency check by	L. Fonseca, G. Arthur	30/08/2010	All
Approved by	Coordination Board	24/11/2010	All

Document Log

Issue	Date	Comment	Author
1	20/12/2010	Submitted to EC	MGT

Document Change Record

Issue	Item	Reason Change

TABLE OF CONTENTS

Deliverable D4.8: Definition of Quality Standard for NFFA

1. INTRODUCTION

1.1. Purpose of the document

Purpose of this document is to outline briefly the process which lead to highlight the need and to the subsequent definition of a quality and standard statement for the NFFA research infrastructure.

1.2. Application Area

Targets of this document are the members of the NFFA Project, the EC Project Officers and the general public.

1.3. References

Description of Work (DoW). See at web site:
http://www.nffa.eu/UserFiles/file/Annex_I_DoW.pdf

1.3.1. Objective of Work Package 4

Define the mission and the general structure of the future NFFA-RI, including general management of the central RI and of the local facilities, access criteria via quick international review of projects.

Develop schemes for implementing a NFFA-RI repository of data and protocols and to make it available to the general users. Develop schemes for remote use of NFFA-RI.

Set quality standards of production. Define efficient users' access.

1.3.2. Description of work broken down into tasks

Among the different tasks defined in WP4, this deliverable concerns specifically to:

T4.8) Define the **quality standard for NFFA-RI products and service**. The definition of standards, using the results of metrology, will provide the reference basis for the plan on how to enforce standards in all NFFA-RI Centres, and how to revise and upgrade standards periodically. Quality control of NFFA must include technical definitions (metrology, reproducibility) laboratory procedures for data and management (time to access, peer review) as well as availability of data in the repository in useful form for remote consulting and for remote users, and for interoperability.

2. EXECUTIVE SUMMARY

The NFFA-Research Infrastructure, being an open access distributed facility addressed to a wide basis of customers (the users) and aiming to create a common metrology and protocols platform, will necessarily deal with the "**quality**" and "**standard**" concepts.

The issue of "**quality**" management system (QMS) is mainly treated by the well known ISO 9000 family, essentially based on the concepts of continual improvement of the system and of assurance of conformity to customer and applicable statutory and regulatory requirements. The key rules are:

- to apply the operating PDCA principle that is to **P**lan – to **D**o – to **C**heck – to **A**ct,
- the managing structure must be clear,
- the organization should invite its clients to audit.

In this framework, the users policy plays a fundamental role, and quality rules will need to be implemented mainly for the following three objectives:

- a more flexible access with respect to existing infrastructures, including a strategic access to the analytical LSFs,
- actions to foster access of new users communities,
- implementation of a more effective data management.

Among these, the main quality aspects concerning the newest concept of data management are:

- the data format and the metadata composition,
- IPR issues,
- the effects on users and metausers (users only accessing the Data Repository).

If the Data consist of all the information that the user requested access for, the Metadata is instead the set of "additional" information making the data more widely "useful", beyond the parent user and beyond the time window of the facility operations. In order to achieve the best compromise between a completely free Metadata composition, associated with a semantic search criterion (which is more flexible but less inclined to smart application forms and analysis), and a set of keywords (very effective for widespread software applications but more affected by versioning problems), a hybrid system will be adopted.

IPR issues will be mainly based on a user request strategy associated with an *ex-post* evaluation, in order to avoid stringent fixed rules which may act as a bottleneck.

Whenever an access request to read or download data or protocols from the NFFA data repository will take place (all such actions will be recorded), external metausers will be asked to accept copy right conditions.

A "**standard**" provides rules and/or characteristics for activities or for ensuing results aiming at common and repeated use. As the nanoscience competence core is still mainly shared among scientific institutions which have not an adequate involvement/interest in the normative activity, as manufactures and entrepreneurs typically have, any effort towards establishing more common practices and round robin activities that aim at comparing processes and results at the atomic scale among scientific research groups, will push forward the implementation of more effective standardization assets.

New phenomena have emerged at LSFs by exploiting extreme conditions of sources and sample environment so that advanced programmes are strongly dependent on the availability of advanced and reliable metrology. Measurements must be compared with each other and this requires that absolute values of key parameters are known, within well established and routinely verified error bars.

Also the sample preparation, characterization and the parameters of the sample environment must be certified by an appropriate reliable metrology. There is a need at LSFs to overcome waste of time in reproducing time-consuming sample preparations, difficulties in comparing quantitatively complementary techniques available at different sites, and the critical level in performing *in-situ* or *in-operando* measurements. This need can be overcome by two actions of "common" practice.

First, an internal common **standard of protocols** which can be facilitated by technical solutions implemented directly at the LSF site or in conjunction to the nearby NFFA site, that physically link time-consuming sample preparation to analytical beamlines: for instance by implementing sample transfer under UHV controlled conditions or by directly connecting synthesis chambers to the beamlines, where appropriate, or by implementing EM-field manipulators for cells or macromolecular assemblies, with known applied pressure.

Second, an internal common **standard of metrology**, aiming at exploiting the link between fine analysis and atomic scale manufacturing/characterization at different complementary sites, and where all the physical, chemical and morphological parameters are under full control and quantified with the proper uncertainty.

Finally, the internal common **standard of data**, as described above, will be the means making protocols and metrology standards readable, reachable and transferable.

Common standards and data management are therefore the actions that can upgrade the very valuable arsenal of European Large Scale Radiation Facilities for Fine Analysis.

The **implementation** of common standards will require technical as well as organizational solutions like the correct estimate of duty cycles in the equipment time, an adequate involvement of the staff personnel and data-metadata management meeting specific requests concerning metrology and protocols (e.g. the reference to calibration operations).

For such a purpose, the **NFFA Technical Liaison (TL)**, a coordinated activity which aims at managing the technical competences, by acting in:

- Common metrology and protocols,
- Data Repository management,

which are two of its competence areas, will guarantee an adequate level of round robin activity for establishing internal standards and for performing quality checks and calibrations and the proper level of control/coordination of the quality data management. Indeed the TL engagement, beyond the assistance of inexperienced users, aims basically to avoid a spontaneous and non coordinated participation to the implementation and the operations of two of the fundamental points of the NFFA vision: the common platform of protocol and metrology standards, and the Data Repository.

A particular **recommendation** concerns a reliable implementation of this common platform, which is upfront mandatory in order to maximize the success of the NFFA initiative. This means to include:

- a kernel of instruments specifically devoted and adapted for common metrology and protocols,
- a kernel of personnel specifically in charge for the Technical Liaison objective,
- virtuous and well defined (internal) standardization, technical development and data management activities linking the two throughout all the NFFA centres.

On the other side, widespread instrumentation and personnel shared with the participant institutions within a more relaxed agreement are well suited for conducting users as well as in-house experiments and carrying out a massive part of the NFFA scientific programme.

3. BACKGROUND

The Council of the European Union adopted the Council Conclusions on Standardization and Innovation in March 2009[1] in considering "*the essential contribution which standardization can make towards developing innovation and competitiveness, by facilitating access to markets, enabling interoperability between new and existing products, services and processes, enhancing protection of users, giving consumers confidence in innovations and disseminating research results*". Among its several conclusions was also the recognition that "*both standards and patents are innovation dissemination tools…*".

Though in the past Quality and Standards in the research field had not been relevant for a wide range of activities (from individual research groups at universities or public institutions to Large Scale Facilities), nowadays such issues are becoming more and more important, in particular whenever interdisciplinary connections, "external" liaisons (new users or industrial customers) as well as funding supports are concerned. An adequate level of both Quality and Standards will be thus necessary for a research infrastructure operating in the nanotechnology related fields, aiming to offer open access to wide scientific and technological communities and to establish a boost toward the atomic scale manufacturing and characterization capabilities which, if effective, will be the seed for widespread applications, services and industrial innovation.

The NFFA Design Study (DS) has indeed a multifaceted connection with standardization mainly due to two aspects:

- It is an **open access facility addressed to a wide basis of customers** (the users), coming from scientific, technological, industrial and services communities related to micro- and nano-products and atomic scale manufacturing. It is therefore obvious that NFFA will aim to meet and satisfy these

potential users in terms of both technical and management aspects in such a way to foster development and innovation.

- It aims to create a **common platform of standard and protocols** by integrating, with different levels of actions, the complementary instruments inside each NFFA centre, the several distributed NFFA centres and the associated analytical LSFs.

The first aspect is more related to the term "**Quality**" (or quality standard) which usually refers to standards in the management system, which are process standards and not product standards, while the second aspect is associated to the generic term "**Standards**", which typically refers to products, specific of market sectors or technological areas.

Here is the need, that is the aim of the present document, first, to address the adequate level of Quality and Standards that the distributed NFFA-Research Infrastructure (RI) will have to satisfy and, second, to deepen possible developments in terms of certifications, that specific activities or specific NFFA centres, should meet as special/local needs or opportunities. In the following chapters, mainly those aspects of quality and standards that need constant monitoring and improvement will be analyzed, being this self-organization action the most established method of quality concept. The document intends therefore to give clear indications on what the quality management system should include and what the internal common standards should address.

4. CURRENT STANDARDIZATION ISSUES

A standard provides rules and/or characteristics for activities or for ensuing results, aiming at **common and repeated use**. The aim is to achieve the best degree of order.

Worldwide, three bodies are responsible for the planning, the development and the adoption of International Standards: **ISO**, the International Organization for Standardization is responsible for all sectors except for the Electrotechnical field, which is the responsibility of **IEC** (the International Electrotechnical Committee), and most of the Telecommunications Technologies, which are largely the responsibility of **ITU** (International Telecommunication Union). ISO is a legal association, whose members are the National Standards Bodies (NSBs) of about 158 countries (organizations representing social and economic interests at the international level), supported by a Central Secretariat based in Geneva, Switzerland. The main deliverable of ISO is the International Standard.

The procedure of delivering a standard is quite long and complex since it requires several feedbacks of consensus and acknowledged technical approvals. Intermediate documents such as Technical Specifications (TS) or supporting documents such as Technical Reports (TR) are anyway published.

Application of ISO standards is voluntary. ISO is a non-governmental organization and has no power to enforce the implementation of the standards it develops. Constituting therefore a technical basis, the standards can be eventually implemented in regulatory frameworks by public authorities.

At European as well as at national levels, other organizations operate. At European level for instance CEN (European Committee for Standardization) has a specific mandate from the EC.

4.1 The state of the art in quality standard

ISO standards providing requirements or giving guidance on good management practice are among the best known of ISO's offering. The issue of **quality management system** (QMS) is mainly treated by the well known ISO 9000 family, developed by the ISO/TC 176 Technical Committee. It addresses what a generic organization does in order to fulfil:

1. the customer's quality requirements, and
2. applicable regulatory requirements, while aiming to
3. enhance customer satisfaction, and
4. achieve continual improvement of its performance in pursuit of these objectives.

In the ISO 9000 family, guidelines giving fundamentals and vocabulary of QMS are published, as well as the ISO 9001 standard, providing requirements that an organization has to fulfill in order to obtain the quality certification. The most recent version of the ISO 9001 is the ISO 9001:2008 which specifies requirements for a quality management system where an organization

- needs to demonstrate its ability to consistently provide a product that meets customer and applicable statutory and regulatory requirements, and
- aims to enhance customer satisfaction through the effective application of the system, including processes for **continual improvement** of the system and the assurance of **conformity** to customer and applicable statutory and regulatory requirements.

The essential QMS is schematized in fig. 1 and can be roughly summarized in the following concepts:

- the operating principle is the Plan – Do – Check – Act (PDCA) cycle. Therefore (1) **establishing objectives** and making plans, (2) **implementing** them (doing what has been planned to), (3) **measuring** the results and how far they are from planned objectives, (4) **correcting** and improving plans (mistakes as feed back to improve);
- the organization must retain full control of its activities, including an effective traceability of events;
- the managing structure must be clear and all the people involved in the organization activities must be well aware of it;
- the organization should invite its clients to audit, but avoiding multiple audits or reducing the frequency or duration of client audits.

All requirements of ISO 9001:2008 are generic and are intended to be applicable to all organizations, regardless of type, size and product provided.

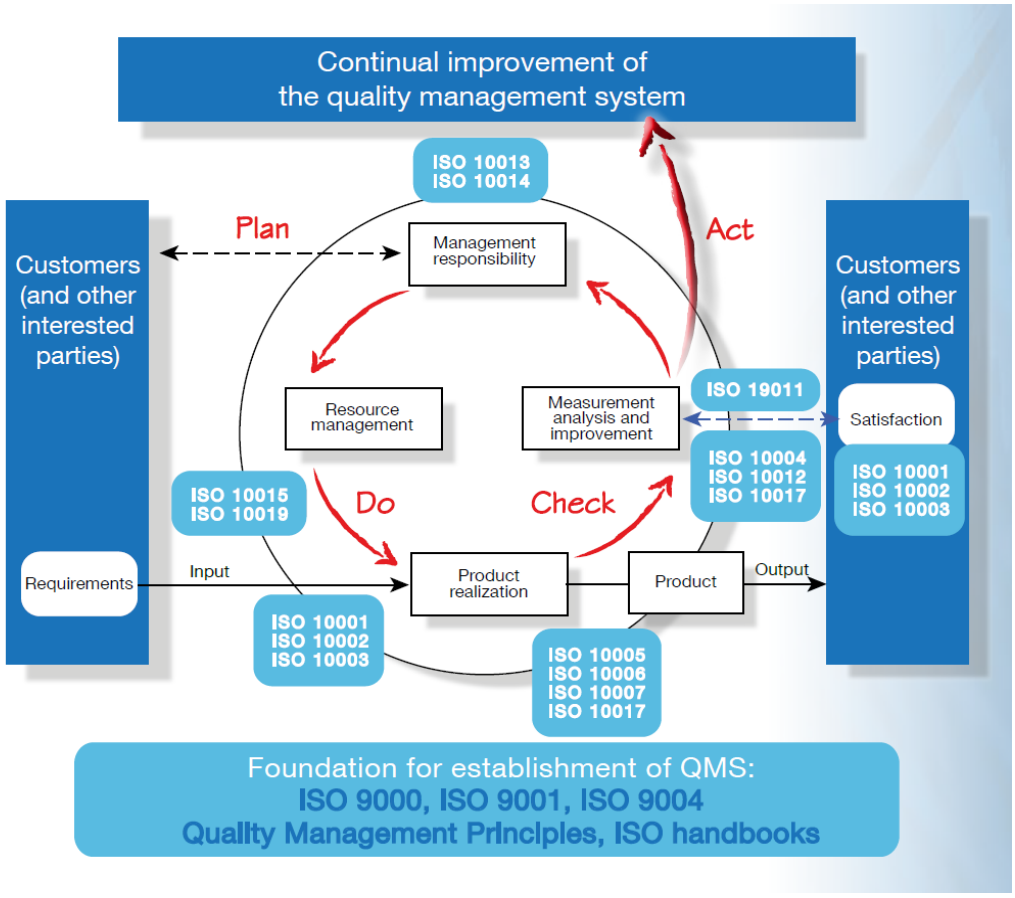

Fig. 1 Application of ISO/TC 176 standards in the process approach.

4.2 The state of the art in standard normative in nanotechnology related fields

At present, **ISO TC229** (the ISO Technical Committee devoted to nanotechnology and established in 2005) in liaison with IEC TC 113, are steering the activity at the international level on nanotechnology standards. Its business plan has been delivered on April 20th 2010 (ISO/TC 229 N706). Other standard bodies, which started to work on nanotechnology a couple of years in advance, like several other ISO Technical Committees (TC), national standards bodies and Standard Developing Organizations such as ASTM and IEEE, are in liaison with ISO TC229 and IEC TC 113; likewise CEN, CENELEC and ETSI that operate with a specific mandate from the EC. The map sketched in fig. 2 gives an idea of the complex scenario in which nanotechnology related stuffs are involved and connected with.

ISO TC 229 is structured in 4 Working Groups (WG) focusing on crucial issues for the development of an effective regulation for nanotechnology-related products. These are:

- Terminology and Nomenclature
- Measurements and Characterization
- Health, Safety, and Environment
- Materials Specification

A more detailed panoramic on the state of the art is available from Reports of European projects funded by FP 7 like FramingNano[2] and ObservatoryNano[3] that aim to observe advancements in the field of regulation in nanotech related fields.

So far ISO TC 229 has produced three documents: (1)the ISO/TS27687 (Technical Specification: Terminology and definitions for nano-objects - Nanoparticle, nanofibre and nanoplates), (2) the ISO/TR 12885 (Technical Report: Health and safety practices in occupational settings relevant to nanotechnologies) and (3) ISO/TS80004-3 (Technical Specifications: Vocabulary-part 3: carbon nano-objects). This fact shows significantly that nanotechnology and atomic scale standardization activity is still at a very early stage and it is not running in a proper established manner and with an effective timing with respect to the market requests. As a matter of fact, very recently the BSI (British Standards Institution) informed CEN of its intention to relinquish the secretariat of CEN/TC 352[4]: *"Much of the effort of TC 352 over the last three years has been in the expectation of a mandate from the EC for nanotechnologies standardization"* finalized at the beginning of 2010[5].

Although facing a huge increase of on-the-market materials which are structured at the nanoscale level, the main bottleneck in nanotechnology standardization has been addressed to be the lack of common spaces where an effective feedback on regulation is driven. Such common spaces should be not only technical platforms based on common competences but also effective organizational spaces where characterizations (also from the point of view of environment and toxicity) take place with an adequate practice in terms of quantitative values and uncertainties as well as in response time. The critical point is that a so quick throughput, as we have at present, of applications and products directly delivered by scientific results and scientific institutions, capable of tracking a new paradigm of the development-to-market innovation chain has never been achieved in the past. This means that new nano-products potentially ready to the market are indeed less based on commonly established technological platforms and regulation frameworks, than products obtained by more conventional technologies were in the past, when legislative competences were sufficient to meet widespread technical competences transferred from public institutions to private industries and SMEs. In other words, in the case of nanotechnology the competence core is mainly shared among scientific institutions which have not an adequate involvement/interest in the normative activity as manufactures and entrepreneurs typically have.

Any effort pointing to establish more common practices and round robin activities aiming at comparing, among scientific institutions, processes and results at the atomic scale, will push forward in implementing more effective standardization assets.

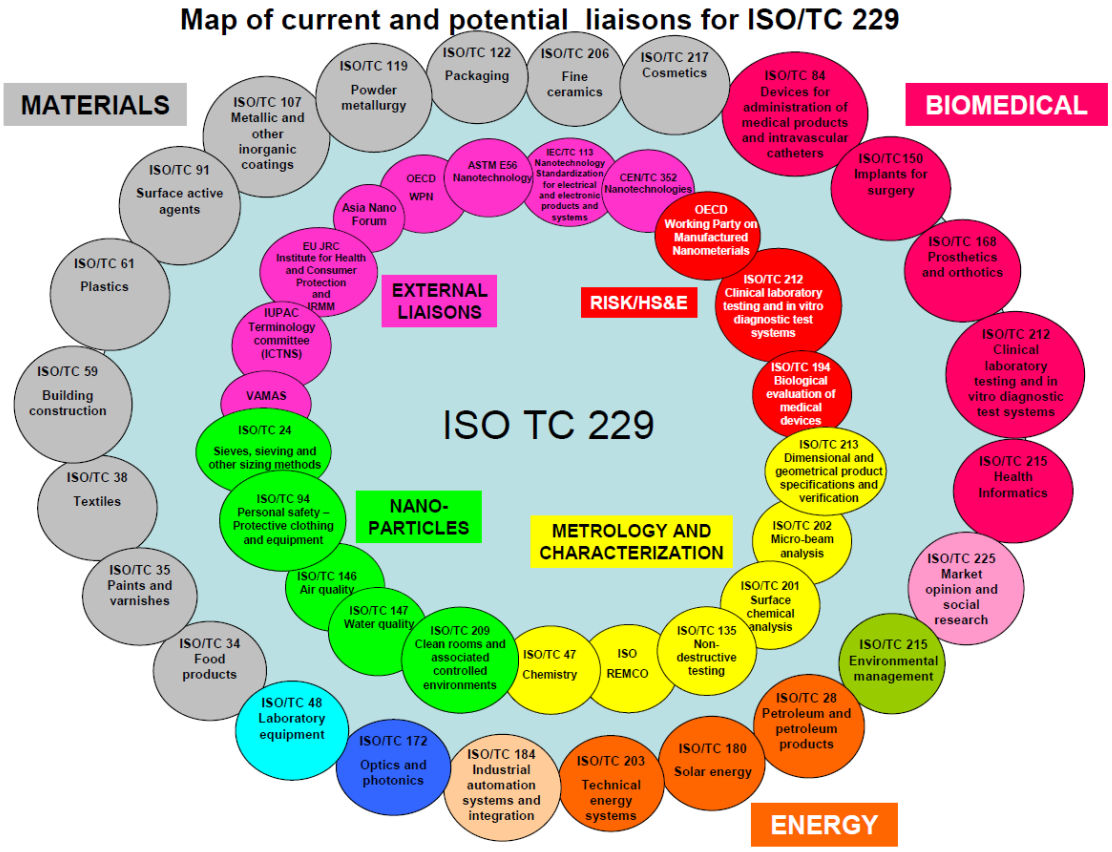

Fig. 2 Potential liaisons of ISO/TC 229

5. THE NEED FOR QUALITY STANDARDS FOR THE NFFA CENTRES

The heterogeneous composition in terms of competences, facilities and users communities of a research infrastructure - as the NFFA-DS has been planning to design - makes an adequate standard of quality mandatory, in order to deal with complex but flexible access and scheduling, complex but effective proposals and experiments, and complex but smart and useful data. Nonetheless a distributed infrastructure, i.e. physically located on different sites in different member states but having to operate as a single portal, effectively connected with the associated analytical LSFs, will need a step forward in terms of organization relaying on simple and well established rules in an attempt to avoid an unnecessarily complex organization.

5.1 Quality management at NFFA

Quality management adopts eight management principles that can be used by upper management to guide their organizations towards improved performance[6]. The principles cover:

- Customer focus
- Leadership
- Involvement of people
- Process approach
- System approach to management
- Continual improvement
- Factual approach to decision making
- Mutually beneficial supplier relationships

To study such principles in details or to outline a management system that fulfils all of the requirements concerning these principles is out of the scope of the present document. Instead, by highlighting some of these aspects in connection with the NFFA strategy, it is essential to assess final remarks concerning the quality standard well suited for the NFFA-DS.

Customer focus: (organizations depend on their customers and therefore should understand current and future customer needs, should meet customer requirements and strive to exceed customer expectations). This important issue will be treated in the next section.

Leadership: (leaders establish unity of purpose and direction of the organization. They should create and maintain the internal environment in which people can become fully involved in achieving the organization's objectives). Inside the NFFA infrastructure, responsibilities have to be well defined at all levels in order to manage a complex infrastructure located at different sites, where several internal facilities and several facilities of the associated Analytical LSFs, all of these under the management of heterogeneous groups and institutions, have to operate together in a complementary way on the same experiments.

Involvement of people: (people at all levels are the essence of an organization and their full involvement enables their abilities to be used for the organization's benefit). This is a peculiar issue whenever people of several institutions are asked to join in a common mission. Scientists in research infrastructures are typically asked to provide a certain quota of its employment for facility operations and free to use another quota for his own research. An adequate involvement and motivation will then be fundamental to guarantee the proper level of participation in all the NFFA operations, including management activities and satellite activities related to users and proposal processing. A satisfactory balance between what a single researcher will benefit by the NFFA-RI and what he is asked to provide to, is therefore necessary.

Process approach: (a desired result is achieved more efficiently when activities and related resources are managed as a process). If the activities are managed as a process, it is easier to shorten cycle times, to share synergies, to schedule accesses and to give a simple and clear view of the “process” to the user.

System approach to management (identifying, understanding and managing interrelated processes as a system contributes to the organization's effectiveness and efficiency in achieving its objectives). Once again, due to the fact that the NFFA activities are not characterized by a single component competence (single instrumentation, single laboratory, single beamline) as is typically the case for instance at the analytical LSFs, a process approach will help multi-technique and multitasking activities at the NFFA centres.

Continual improvement (continual improvement of the organization's overall performance should be a permanent objective of the organization). Due to the novelty level of the NFFA-RI it is reasonable that, particularly at the beginning, activities and their interconnections will be steered as a self-organization process. It is therefore important to implement audit and feedback operations in order to get as soon as possible an adequate level of quality, and to maintain the capability to improve according to the users and scientific needs that will not necessarily stay constant in the future.

Factual approach to decision making (effective decisions are based on the analysis of data and information). Taking the advantage of the opportunity of setting up a reliable data repository, information concerning the accomplishment of users needs and scientific tasks could be integrated in data and metadata of NFFA experiments, allowing for a more factual decisions. As a matter of fact, scientific evaluation can be at present performed only on published data, but it is well known that there is a sizable amount of unpublished or off-centre data which have a potential exploitation, in particular in the frame of a virtuous cycle of procedures and protocols refinement. The data repository will then aim also to recycle dormant data.

Mutually beneficial supplier *relationships* (an organization and its suppliers are interdependent and a mutually beneficial relationship enhances the ability of both to create value). As the correct involvement is peculiar of individual people, likewise mutually beneficial supplier relationships is the basis for a reliable cooperation of different institutions participating to a common mission. The respective agreements, their

implementation and the mutual added values (the common platform and the link with complementary LSFs among the several NFFA centres, the exchange of technical-scientific support and users with the LSFs) will be then of primary relevance for the success of the NFFA-DS implementation.

5.2 Users policy

From the point of view of the typical customers (the users) the NFFA policy will be characterized mainly by three aspects:

- a **more flexible access** with respect to typical periodic access experienced by most of the existing research infrastructures, including a strategic access to the LSFs;
- actions to foster access of **new users communities** by exploiting the joint venture between nanoscience and nanofabrication tools and the fine analysis available at the LSFs;
- implementation of a more **effective data management** in all of the access steps: proposal application and evaluation (including a possible technical support in going from an idea to a work planned proposal), data storage, analysis and dissemination among collaborators during the facility operations and, subsequently, data repository and publication for open access of standard protocols and data.

Whatever the user access will be, as described in Deliverable D4.4, a good management system is mandatory in order to guarantee a high quality standard. This means including for the three aforementioned aspects the corresponding audit feedbacks: in particular, an audit by registered users in order to verify the quality of operations at the NFFA centres, an investigation on new potential users in order to verify if new interests in the NFFA capabilities are seeding in some specific fields of technological innovation and high-tech manufacturing and services and, finally, the implementation of some evaluation tools in the data repository both from the point of view of the user as well as from the point of view of the external visitors (“metausers”) that access the data repository by using search engines handling mainly with “metadata”, in order to acquire information on standardized data and protocols.

A continuous activity of analysis and improvement of the users access in terms of timing, scheduling and users flux through the NFFA facilities is fundamental in order to optimize the user operations path, seen as a process (which eventually becomes a software application from the point of view of the data repository, see D4.9), and in order to maximize the exploitation of the NFFA facilities and of the associated analytical LSFs as well.

Finally, the effort made to provide technical assistance to inexperienced users has also to be verified, qualitatively and quantitatively, and properly sized with respect to the whole NFFA activity.

5.3 Data management: quality standard of the data repository and IPR issues

In the frame of the “common” concept concerning metrology, protocols and procedures standards, that is in sharing and effectively quantifying, comparing and calibrating technical tools, a key role is played by the methodology and policy of storing and exchanging data.

It is important to highlight few main aspects concerning the quality of data management:

- the data format and the metadata composition,
- IPR issues,
- the effects on users and metausers.

The first aspect will be treated in the following section.

IPR (Intellectual Property Rights) issues are notoriously important and tricky as well. One of the bottlenecks of existing facilities is just the long time and heavy bureaucracy of IPR issues when dealing with private companies. For both non proprietary and proprietary research a NDA (Non Disclosure Agreement) will be guaranteed by the NFFA structures(User Administration, Advisory Panels, Technical Liaison, facility research staff, etc.) involved in the idea/proposal processing and the proposal will be tracked by a temporal mark testifying the temporal allocation of the specific idea. The proposal format (User identity, requested techniques and competences, Metadata keywords, etc.), together with all the subsequent data/metadata

entries in the repository will act as an internal criterion to manage priority access and data publication rights. The parent user is free to use all the information for his own interest. Subsequently the main IPR criterion is based on a user request basis, in case evaluated ex-post, trying to avoid stringent fixed rules which may act as bottleneck (for more details see the D4.9 on Data Repository).

Instead, from the metauser point of view, whenever an access request to read or download data or protocols from the NFFA data repository will take place, the external user will be asked at any time to accept conditions in order to properly refer to the source and its property rights in whatever use of the NFFA data will be made.

In order to satisfy an adequate level of quality data management, any operation on the data repository, data entry or output request, will be recorded on the data repository and the user/metauser will be identified.

A very important quality issue of data management is how data format, metadata composition, search criteria and IPR issues will affect the users. The key point to highlight is that all the data management must be as little invasive as possible on the users activities. Therefore automatic procedures have to be implemented whenever it will be feasible, in particular referring to automatic storage by the instrumentation. Once again, in virtue of the quality system concept, proper audit feedbacks must be implemented toward users as well as metausers, in order to optimize, respectively, data input during facility operations and data output for disseminating results and making them more promptly available for applications and interoperability.

6.THE NEED FOR COMMON STANDARDS ON PROTOCOLS, METROLOGY AND DATA FOR THE NFFA DISTRIBUTED INFRASTRUCTURE

Advanced science experiments often demonstrate new phenomena by exploiting extreme conditions of sources and sample environment. The Large Scale Facilities, as they are operated today, are well suited for such experiments that are then generally published on high impact journal and stimulate further efforts for reaching new understanding at the phenomenological level. Science development programmes, like materials science, are also tributary of systematic work where advanced, well established, probes are applied systematically on materials grown in modified conditions, or subject to thermal, pressure, field treatments, and possibly with *in-situ* and *in-operando* conditions. This scientific activity is strongly dependent on the availability of advanced and reliable metrology. The measurements campaigns must be compared with each other and this requires that absolute values of key parameters (radiation intensity, degree of polarization, focus dimension, degree of coherence, monochromaticity…) are known, within well established and routinely verified error bars.

Also the sample preparation, characterization and the parameters of the sample environment must be certified by an appropriate reliable metrology.

Under the above conditions research will benefit from the full impact of large scale facilities, since data will be obtained on comparable samples, in quantitatively comparable conditions, and with enough quantitative information to directly feed information and constraints into the overall data analysis and finally interpretation work.

Metrology and data management are the two actions that can upgrade the very valuable arsenal of European Large Scale Radiation Facilities for Fine Analysis, into a truly unique asset in the development of science and technology. These aspects are addressed within the NFFA DS.

6.1 Internal common standard of protocols to join sample synthesis and definition with fine analysis at the LSFs

The need to enhance sample definition capabilities originates from some aspects characterizing an underachieved exploitation of analytical LSFs occurring mainly in the field of modern material science:

- in allocated beamtime for the fine characterization of complex samples for which a capping-decapping procedures to preserve its characteristics is not available and whose synthesis (typically a time-consuming procedure) has been developed at home by the users, most of the beamtime is lost to correctly reproduce the same synthesis;
- the same reproducibility problem is even more serious if a comparison among complementary techniques available at LSFs located at different sites has to be achieved;
- similar reproducibility or normalization problems affect analytical results whenever in-situ or in-operando measurements have to be carried out.

In such circumstances, the capability to improve the understanding of processes governing synthesis (self-assembly is the emblematic case), , a challenge which is more and more faced in the field of hybrid interfaces (with biological, organic and inorganic materials), multilayers and nanostructured functional materials, is dramatically suppressed. It is therefore desirable to have well established technical solutions as well as properly organized access to overcome this drawback, which constitutes a real bottleneck for the development of new complex functional materials.

A first possibility to improve sample definition is to join synthesis and nano-assembly facilities with fine analysis facilities, in the same site, in order to facilitate technical solutions that physically link time-consuming sample preparation to analytical beamlines; for instance implementing sample transfer under UHV controlled conditions or directly connecting synthesis chambers to the beamlines. On this basis it is essential to push for the establishment of well defined protocols, as an internal standard to be validated and commonly used, to make procedures reproducible and, at least, comparable in a quantitative way. This means that all the physical and chemical parameters must be under control and quantified with the proper uncertainty. In order to make such a practice to become a common added value, beyond a single user and single site scenario, a quality methodology has to be implemented, that is, in a self-organizing manner, planning some objectives, implementing them in a defined time window, measuring the results and acting with feedback corrections. All of these phases have to be well documented and supported by specific technical reports. Finally, those common procedures for sample synthesis, characterization and transfer have to be implemented and made available in the data repository.

6.2 Internal common standard of metrology to exploit the link between fine analysis and atomic scale manufacturing/characterization at different complementary sites

A second solution to improve sample definition is to establish a common metrology, shared among the several NFFA centres and with the associated analytical LSFs, aiming to define in an as much absolute as possible way the samples, synthesized and characterized at different sites, in order to make quantitative comparisons feasible and to make the information transferable from one measurement to another. This means that all the physical, chemical and morphological parameters have to be under control and quantified with the proper uncertainty and all the techniques like microscopies and spectroscopies have to give as much as possible absolute information characterized by the proper error bar. This will allow the user to properly quantify at least the “difference” of the achieved sample definition, for instance whenever the same exact synthesis or fabrication procedure will not be feasible at different sites. Another need is to make transferable the sample definition from typical samples of the order of micrograms in synchrotron radiation investigations to typical samples of the order of milligrams in neutron investigations; this will allow the transfer of complementary information to be quantitatively reliable. This common metrology strategy will also meet a known demand of the private industries[7], which are requesting for more “absolute” numbers and less “relative” intensities and peaks coming out from spectroscopies and structural characterizations.

The implementation of such a common metrology will require technical (more details are given in the Deliverable D3.4) as well as organizational solutions. It is clear that specific efforts, in terms of equipment time, personnel and data management as well, have to be taken for setting up an effective and reliable system. This means that duty cycle time has to be considered for calibrating instruments and carrying out round robin activities aimed at comparing measurements and techniques and at setting up common

procedures and protocols. The associated personnel issues are considered in the section devoted to the Technical Liaison structure.

6.3 A common standard of data to make results more promptly suitable for internal exchange (among the NFFA centres) and for external dissemination

One of the primary goals of the Data Repository design will be systemise data in a suitable way to support the common metrology and protocols target. For instance, the automatic storage of some information concerning the instrument setting, that in principle may be not essential for the data itself, could be instead technically useful for the internal staff for the common metrology implementation (e.g. some physical conditions of tools which are not of direct pertinence of the techniques or of the synthesis principles, like mirrors position, currents, pumping systems and so on). The data format can be then thought so as to meet specific requests concerning metrology and protocols; the uncertainties or the reference to the result of the last calibration operation are an example.

Though the Data Repository concept will be developed in D4.9, some definitions are necessary before assessing quality standard aspects. The **Data** consist of all the information coming out from analysis or characterization operations; roughly, the information that the user requested access for. The **Metadata** is the set of "additional" information making the data more widely "useful", not only for the user that has generated the Data, but also for the metauser that will access the Data, once it will be published for open access on the Data Repository, as well as for the Data itself that will be much more defined in terms of physical conditions and instrumental settings and therefore more unambiguously comparable with other Data.

The Data format and the Metadata composition will affect the data management in terms of accessibility, i.e. readability and transferability, and usefulness, i.e. capability to make the data useful beyond the users that generated it and beyond the time window in which user operations took place. It is then advised to use as much as possible well established standards like HDF format (Hierarchical Data Format), which is widely used due to its capability to save storage memory and to the availability of tools for its conversion into many other formats specific of analysis or simulation applications and codes. This will also permit in the future easier and more reliable connection with emerging e-infrastructures that will be developed for data analysis and dissemination. The Metadata composition, i.e. its capability to return a useful data, will need special attention in the quality system management. If on one side it would be desirable to have the possibility to improve in the future the "quality" of the data management and therefore to think about a upgradable Metadata composition, attention must be paid on the readability and compatibility of "new versions" of Metadata compositions. It is therefore advised to find the correct compromise between the two extreme criteria of Metadata composition and search, that is: (i) a set of keywords making the Metadata ready to play, reliable but less inclined to be flexible, (ii) a completely free Metadata composition associated to a semantic search criteria, making Metadata flexible the but less inclined to be smart in terms of interface and comparison issues. Though an exhaustive set of keywords is recommended even since the beginning, the possibility to add new keywords must be considered, whenever a quality evaluation-feedback cycle or explicit user request will drive it. In order to minimize the "versioning" effect, whenever an old version Metadata will be loaded, it should be upgraded to a new set of keywords which could be identified by means of all the semantic connections with the new available keywords.

This data and metadata common standard will be a further concrete instrument of cross-linking among the NFFA centres and with the associated analytical LSFs. A standard which has to be able to meet as much as possible other standards of emerging e-infrastructures, will allow for a more effective dissemination, even beyond the NFFA Data Repository competence, as an interoperability capacity of the outcome of the NFFA-RI.

It is quite evident that all these aspects, together with what has been mentioned in paragraph 4.3, make the data standard and data quality management system an important item for the success of the NFFA implementation.

6.4 NFFA standard efforts versus pre-normative research and normative activities

On one side it must be clear that normative activities are not included in the mission (cf. Deliverable D4.1) of the NFFA-RI as well as pre-normative research is not a primary priority in its scientific programme (see Deliverable D2.2); there are indeed international organizations (ISO and CEN) and national metrology institutes, respectively, having such objectives. On the other side, it is true that NFFA centres will spend some effort in creating and maintaining for internal use common quality standards of metrology and protocols. It is therefore true that a bilateral relationship could be established as a reciprocal added value. In fact in one direction, existing normative, if any, can be used to easily set up metrology procedures and synthesis protocols, referring totally or partially to published and internationally approved standards. In the other directions, actions made by the NFFA centres concerning internal common standardization, could be made available to normative activities, not only as a public result (for instance available in the data repository) but even in terms of NFFA personnel, participating to the Technical Committees of the organizations in charge or carrying out round robin measurements on their behalf. This is of course a spontaneous involvement, but one well suited to technologists devoted to the quality and standard management. As a matter of fact, the author of the present document is member of the Technical Committee U22-Nanotecnologie of UNI (the Italian institution for standardization).

Another possibility is that NFFA-RI, as a corporate body, participates to associations devoted to pre-normative research like, for instance VAMAS (Versailles Project on Advanced Materials and Standards[8]) which was conceived in 1982 following a ”G7” economic summit. Its main objective is to support trade in high technology products, through international collaborative projects aimed at providing the technical basis for drafting codes of practice and specifications for advanced materials. The scope of the collaboration embraces all agreed aspects of science and technology concerned with advanced materials, including materials technology, test methods, design methods and materials databases that are required as a precursor to the drafting of standards. VAMAS activity emphasises collaboration on pre-standards measurement research, inter-comparison of test results, and consolidation of existing views on priorities for standardisation.

Indeed, facing technical difficulties of the Technical Committees to carry out normative actions in the complex field of the nanotechnologies, such a relationship between the NFFA-RI and standardization institutions, could enable a more effective and safer dissemination of nano and atomic scale related products and services.

6.5 The role of the Technical Liaison

The NFFA Technical Liaison (TL), defined as the structure managing the technical competences (see D4.3 on Scientific Management), will act in the following areas in a cross-party way among the several NFFA centres:

- Users access (scientific and technological support to inexperienced users, so including ILO activity and promotion of collaborations),
- Common metrology and protocols,
- Data Repository management,
- Local Desk Service (like short time characterization by microscopy and spectroscopy),
- Characterization of associated LSF methods and development of technical solutions to link nanoscience instrumentation at the NFFA centres with analytical methods at the associated LSFs.

For what quality and standard may concerns, that is mainly the second and the third points, the TL activity will help to guarantee an adequate level of round robin activity for establishing internal standards and for performing quality checks and the proper level of control/coordination of the quality data management. Indeed the TL engagement, beyond the assistance of inexperienced users, aims basically to avoid a spontaneous and uncoordinated participation to the implementation and the operations of two of the fundamental points of the NFFA vision: the common platform of protocol and metrology standards, and the Data Repository.

Whenever a procedure will be ready to become a common (internal) standard, a round robin activity could be necessary and, finally, an adequate data/metadata format must be taken into account to publish the standard in the Data Repository. This will be a duty of the facility staff involved in the TL, operating at the several NFFA centres. In this way they will enhance their technical knowledge on the NFFA-RI capabilities and they will exchange information on the Data Repository management.

They also will approve a new "keyword" for the Data Repository, whenever a request will be made by a user or by the NFFA staff, verifying afterward the proper interoperability with the Data Repository assignments with respect to proposal forms, data format and technical liaisons.

7. POTENTIAL NFFA CERTIFICATIONS

As outlined above, the NFFA common platform of standards and protocols will be essentially an internal need that does not require formal certification. Anyway there can be specific needs of acquiring formal accreditation at local or at distributed level as well, that have to be dealt with at the proper time. Certifications are delivered by "accreditation" bodies; there are several at national and European level. Among these the EA (European cooperation for Accreditation, operating under the umbrella of the ILAC - International Laboratory Accreditation Cooperation) which is the European network of nationally recognized accreditation bodies located in the European geographical area. Among the accreditations covered by EA there are accreditations of Laboratories (Testing, Calibration), Quality Management Systems, Products and Services. The main standard used by testing and calibration laboratories is the ISO/IEC 17025 that was initially issued by the ISO in 1999. There are many commonalities with the ISO 9000 standard, but ISO/IEC 17025 adds the concept of competence. The two main sections in ISO/IEC 17025 are therefore Management Requirements and Technical Requirements. Management requirements are primarily related to the operation and effectiveness of the quality management system within the laboratory. Technical requirements include factors which determine the correctness and reliability of the tests and calibrations performed in laboratory. Laboratories use ISO/IEC 17025 to implement a quality system aimed at improving their ability to consistently produce valid results. It is also the basis for accreditation from an Accreditation Body. Since such a standard is about competence, accreditation is simply formal recognition of a demonstration of that competence.

7.1 Special issues for industrial/proprietary research

The capability to certify quality standard or specific technical standards related to laboratory measurements is becoming more and more common inside research institutions. Although a quality standard in line with the ISO 9000 guideline is advised in all the activities of the NFFA-RI, the ISO 9001 certification could be relevant whenever external liaisons with private institutions take place. In this view, the Industrial Liaison Office (ILO) could be ISO 9001 certified. This possibility on one side will meet a need that is more frequent among industries, as a guarantee form on a return result upon a formal and paid request, but on the other side will require a bigger effort by the NFFA infrastructure. The final decision will depend upon a correct estimation of benefits and drawbacks, both at local level of the specific centre and at distributed level of the entire infrastructure. It must be taken into account that, in the case of ISO 9001 certification of the ILO, indeed all the activities connected to the ILO have to be involved in the quality certification; for instance also the Technical Liaison structure will be involved as well as all the governance bodies and the management structures connected with the ILO.

7.2 Certification for specific/local needs

In response to specific needs mainly related to local requirements of nearby institutions connected to a particular NFFA centre, a standard certification for some laboratory measurements or manufacturing processes could be well suited inside the NFFA mission and scientific programme. It is clear that there will be no conflict with the internal standard activity of the NFFA distributed infrastructure, on the contrary

such a circumstance will provide a benefit at the NFFA setting. In such a case a direct link with pre-normative research and normative activity, as sketched in paragraph 4.4, is more natural and more fruitful. It must be anyway kept in mind that such a choice has not to affect the capabilities in terms of flexibility of the technical approach which must characterize a scientific infrastructure; therefore there should be a distinction, in terms of personnel and rules, between certification of the service and scientific needs. In this context, once again, the Technical Liaison will play the fundamental role on the certified service side.

8. RECOMMENDATIONS

Due to the novelty of such quality, standard and data management aspects as well as of the common metrology and protocols concept, which are not typical of scientific environments but are peculiar of the NFFA-DS, whatever the NFFA roadmap will be, it is fundamental to claim that a reliable implementation of these common practices is upfront mandatory in order to guarantee the success of the NFFA initiative and effectively meet the NFFA vision. It is therefore essential to implement

- a kernel of instruments specifically adapted for common metrology and protocols,
- the proper amount of sufficiently dedicated personnel to achieve the aforementioned Technical Liaison objectives,
- virtuous and well defined (internal) standardization, technical development and data management activities linking the two.

In such a high quality common platform, which can be “confined” to well selected competence areas, it should be better to include instruments and people which, even if shared with the participant institutions, are involved in the NFFA mission by at least a critical amount of about 60-70 %. The best choice should be to have new instruments (the same ones at the different sites, furnished with the proper customization for satisfying the needs of the Data Repository link and of the calibration operations) and people employed or in charged specifically for the Technical Liaison. In other words, the proper technical effort necessary to put different instruments to be quantitatively comparable (calibrations, procedures, environment control, etc.) and well suited for interoperability with the other facilities in order to satisfy the desired protocols, as well as the complexity to manage people involved in other demanding objectives in different institutions and heterogeneous research groups must be adequately taken into account. The right combined solution is therefore to have a kernel of instrument and personnel mainly devoted to the NFFA common platform, while widespread facilities and personnel shared with the participant institutions, are well suited for conducting users and in-house experiments and carrying out a massive part of the NFFA scientific programme.

9. REFERENCES

[1] delivered by the Council of the European Union in Brussels on 25 September 2008, http://ec.europa.eu/enterprise/policies/european-standards/files/standards_policy/standardisation_innovation/doc/councilconclusions_20080925_en.pdf

[2] http://www.framingnano.eu/

[3] http://www.observatorynano.eu/project/

[4] Document CEN/TC 352 N 138 on June 14th

[5] Document CEN/TC 352 N 133 Rev on February 1st

[6] www.iso.org/iso/iso_9000_selection_and_use-2009.pdf

[7] Conference by ERF (European association of Research Facilities) on: Future Access to European Research Infrastructures: Benefits to Academia, Industry and Society, Lund, 27th October 2009, Parallel Session: Open-private access conditions. http://www.europeanresearchfacilities.eu/ERF_Seminar_20091027.aspx

[8] http://www.vamas.org