International initiative on x-ray fundamental parameters

Objectives of the EXRS2012 event

- Dissemination of information on the 2010 and 2011 workshops (LNE & NIST)
- Presentation of expert groups and road map documents
- Industrial and other FP project activities
- Implementation of new expert group structure
- Continuation of a joint project and follow-up activities

International initiative on x-ray fundamental parameters

Motivation

- **Parameters useful for quantitative x-ray analysis**

  Strong demand of users from many application fields :
  innovative materials, archaeometry, environment, chemistry, etc.

  Tables – reliability – uncertainties ?

  Lack of recent experimental values (few measurements performed >30 years ago)

- **Improvement of experimental facilities**

  Synchrotron, high resolution detectors, improved electronics
  Improvement of calculation speed

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Motivation

- Initiate new measurements taking advantage of technical improvements
- Perform similar measurements in different institutes to establish reliabilty and associated uncertainties of the experimental values
- Perform calculation for selected cases (use calculations for interpolations)
- Compare calculation to experiment
- Provide reliable practical tables to users

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Participants and events

- **Active participation from :**
  - **3 National metrology institutes**
  - **14 Research institutes**
  - **10 Industrial companies**
- **4 international workshops**

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Objectives of the EXRS2012 event

- **Dissemination of information on previous workshops and events**

1st workshop Paris	Oct. 2008	→ definition of expert groups
2nd workshop Berlin	May 2009	→ road map generation
Session at EXRS conf.	Jun. 2010	→ scientific community
3rd workshop Paris	Nov. 2010	→ project options
4th workshop NIST	July 2011	→ definition of new expert groups
prior to EXRS2012	June 2012	→ FP roadmap document online

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Objectives of the EXRS2012 event

- **Presentation of expert groups and road map documents**

1. **Prioritization of FP requirements (energies, elements, uncertainties)**
2. **Experimental facilities (needs for improved instrumentation)**
3. **Theory & codes – challenges: competent use and update of software**
4. **Compilations (need for new strategies), data processing**
5. **Definition of technical terms (NMIs: LNE, NIST and PTB)**
6. **Establishment of a common data base accessible to the public**

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FP roadmap document

Compilation from the work of 6 EG (Roadmap or other shape)

Introduction

EG1: Priorities from the users point of view

EG2: List of available experimental facilities for new experiments

EG3: Theoretical calculations

EG4: Document on the status of databases (publication)

EG5: Technical document : definitions + translations

EG6: Dissemination of the database

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FP roadmap document

Please find the first version of the FP roadmap document at either the **EXSA website** at http://exsa.pytalhost.net/news/?attachment_id=375 or at the **LNE-LNHB website** at http://www.nucleide.org/IIFP.htm

Access to the FP initiative board

The special password protected area can be found at

http://exsa.pytalhost.net/FP-XRF/

with username: xxx and password: xxx

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Objectives of the EXRS2012 event

- **Industrial FP priorities and project activities (“Fribourg group”)**

  → **priorities based on input by industrial manufacturers**

  → **status of industrial FP projects**

- **Extension of competences (input from new attendees)**

  → **new ideas, requirements and contributions**

- **Continuation of a joint project and contributions by regional projects**

  → **discussion and follow-up activities (road map updates, etc.)**

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Objectives of the EXRS2012 event

- **Dissemination of information on the 2010 workshop at LNE, Paris, France**

1 day (November 29, 2010)

Morning session:

Welcome (*M.-C. Lépy)*

Summary of the second workshop in Berlin (*B. Beckhoff)*

Objectives of 3rd workshop (*M.-C. Lépy)*

Burkhard Beckhoff (PTB) "Advanced material characterization and nanotechnology: a novel need for improved fundamental parameters"

Y. Ménesguen (LNE) " Examples of measurements of some FP "

Statement of needs & competences from new attendees

International initiative on x-ray fundamental parameters

Objectives of the EXRS2012 event

- **Dissemination of information on the 2010 workshop at LNE, Paris, France**

1 day (November 29, 2010)

Afternoon session:

Tibor Papp "Specific challenges for FP determination"

Report of expert groups and discussion

Continuing a common project *B. Beckhoff*

Discussion and wish to start a concrete action

Follow-up activities of the FP initiative *T. Jach*

Extension towards USA and Japan

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Objectives of the EXRS2012 event

- **Dissemination of information on the 2011 workshop at NIST, Gaithersb., US**

Day 1 (July 28, 2011) Morning Session

- **Welcome (Terrence Jach)**
- **Introductory Remarks (Michael Mantler),** History of Workshop
- **Tim Elam,** “History of the Elam Absorption Database”
- **Eric Gullikson,** “The CXRO database and Fundamental Parameter Work”

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Objectives of the EXRS2012 event

- **Dissemination of information on the 2011 workshop at NIST, Gaithersb., US**

Day 1 (July 28, 2011) Morning Session

- **Larry Hudson,** “Precision X-ray Measurements at NIST”
- **Matthias Müller,** “X-ray Fundamental Parameter Work at PTB”
- **Jun Kawai,** “X-ray Fundamental Parameter Work in Japan”
- **Jack Glover,** “X-ray Fundamental Parameter Work in Australia”

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Objectives of the EXRS2012 event

- **Dissemination of information on the 2011 workshop at NIST, Gaithersb., US**

Day 1 (July 28, 2011) Afternoon Session

- **Summary of the 3rd Workshop: Marie-Christine Lépy**
- **Objectives of 4th Workshop: Burkhard Beckhoff**
- **Update of Reports of Expert Groups:** discussions and FP roadmap input
- **session devoted to statements of needs & competences from new attendees**

International initiative on x-ray fundamental parameters

Objectives of the EXRS2012 event

- **Dissemination of information on the 2011 workshop at NIST, Gaithersb., US**

Day 2 (July 29, 2011) New business

- **Johanna Hoszowska: report on industry-institution collaboration**
- **New business—revision of expert groups** to reflect completion of some tasks and realignment of others as a result of previous workshops.
- **Proposal for realigned groups:** topics, voluntary chairs and members
- **Final session: decisions on follow-up activities** (road map, new groups)

International initiative on x-ray fundamental parameters

Objectives of the EXRS2012 event

- **Industrial FP priorities and project activities (“Fribourg group”)**

  → priorities based on input by industrial manufacturers

  → status of industrial FP projects

*presentation by **Joanna Hoszowska**, Univ. of Fribourg, Switzerland*

European Metrology Research Programme

EC FP7 EMRP IND07 ‘Metrology for the manufacturing of thin films‘ (2011 – 2014)

Task 1.5: Determination of atomic fundamental parameters for reference based and reference-free X-ray analysis (**PTB,** CEA / LNE-LNHB). Sep. 2012 – Jan. 2014

Aim: The aim of this task is to **substantially improve the reliability of selected atomic fundamental parameters values of matrix elements** relevant to thin film optoelectronics and relied by X-ray measurements

Description of work: **Selected atomic fundamental parameters, such as optical constants, attenuation coefficients, ionisation cross-sections, fluorescence yields and transition probabilities, will be measured.** …. Apart from the optimisation of XRS instrumental parameters for thin-film-stacks, the **reduction of the relative uncertainties of relevant fundamental parameters of selected elements of main interest (Cu, In, Ga, S, Se, Cd, Zn, and Mo)** will contribute to the reliability and uncertainty budget of both reference-based and reference-free analytical techniques. ….

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follow-up workshops and events 2012 to 2014

Recent and current activities:

1st workshop Paris,	Oct. 2008
2nd workshop Berlin,	May 2009
Session at EXRS conf.	Jun. 2010
3rd workshop Paris,	Oct. 2010
4th workshop Gaithersb.,	July 2011
Session at EXRS conf.	Jun. 2012

Scheduled future activities:

Session at DXC conf., USA	Aug. 2012
5th workshop Berlin	Feb./Mar. 2013
Event w. TXRF2013, Japan	Sept. 2013
6th workshop Paris	Feb./Mar. 2014

B. Beckhoff (PTB), T. Jach (NIST) and M.-C. Lépy (LNE)

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Objectives of the EXRS2012 event

- **Implementation of new expert group structure**

1. **Project management and fund raising**
2. **New experimental determinations and methodology**
3. **Theory & codes – challenges: competent use and update of parameters**
4. **Integration of new experimental as well as theoretical parameters into critically evaluated compilations**
5. **Establishment of a common data base accessible to the public**

International initiative on x-ray fundamental parameters

Objectives of the EXRS2012 event

- **Meeting of new expert groups in room MOE58** (max. 20 persons):
  - **Theory & codes – challenges: competent use and update of parameters**
    Monday 16.30 h
  - **New experimental determinations and methodology** **Tuesday 15.40 h**
  - **Integration of new experimental as well as theoretical parameters into critically evaluated compilations** **Thursday 12.30 h**
  - **Establishment of a common data base accessible to the public** **Fr. 10:00 h**
  - **Project management and fund raising** **Friday 10.45 h**

International initiative on x-ray fundamental parameters

Objectives of the EXRS2012 event

- **Meeting of new expert group 3 in room MOE58** (max. 20 persons):
  - **Theory & codes – challenges: competent use and update of parameters**

    Monday 16.30 h
  - **participants:** J. Kawai**,** A. Karydas, St. Fazinić, J. P. Santos, M.-Ch. Lépy, J. Kessler, *and at NIST or DXC2012:* **P. Indelicato, T. Elam**, Z. Chen
  - **presentation: J. P. Santos**
  - **objectives:** setting up a **work agenda**, dissemination to new members

International initiative on x-ray fundamental parameters

Objectives of the EXRS2012 event

- **Meeting of new expert group 2 in room MOE58** (max. 20 persons):
  - **New experimental determinations and methodology**

    Tuesday 15.40 h
  - **participants: M.-Ch. Lépy,** J.-Cl. Dousse, St. Gales, J. Hoszowska, M. Kolbe, J. Kessler, M. Krämer, Y. Ménesguen, M. Müller, B. Beckhoff, M. Rodrigues,…

    and at NIST or DXC2012: **T. Jach,** Z. Chen, J. Gillaspy, P. Indelicato, J. Sieber, V. Samson, D. Sokaras

  - **objectives:** setting up a **work agenda**, dissemination to new members

International initiative on x-ray fundamental parameters

Objectives of the EXRS2012 event

- **Meeting of new expert group 4 in room MOE58** (max. 20 persons):
  - **Integration of new experimental as well as theoretical parameters into critically evaluated compilations** **Thursday 12.30 h**
  - **participants: J. Kawai**, M.-M. Bé, J.E. Fernandez, St. Gales, J.-Cl. Dousse, J. Hoszowska, M. Krämer, T. Papp, *and at NIST or DXC2012:* Z. Chen, J. Glover, Y. Kataoka, V. Kolbytchak, V. Samson
  - **objectives:** setting up a **work agenda**, dissemination to new members

International initiative on x-ray fundamental parameters

Objectives of the EXRS2012 event

- **Meeting of new expert group 5 in room MOE58** (max. 20 persons):
  - **Establishment of a common data base accessible to the public**

    Friday 10.00 h
  - **participants: M. Mantler**, M.-M. Bé, B. Beckhoff, J.-Cl. Dousse,

    J. Hoszowska, M. Krämer, *and at NIST or DXC2012:* B. Cross, J. Sieber
  - **objectives:** setting up a **work agenda**, dissemination to new members

International initiative on x-ray fundamental parameters

Objectives of the EXRS2012 event

- **Meeting of new expert group 1 in room MOE58** (max. 20 persons):
  - **Project management and fund raising**

    Friday 10.45 h *(just after group 5 meeting)*
  - **participants: J. Hoszowska, B. Beckhoff,** J.-Cl. Dousse, M.-Ch. Lépy, Y. Ménesguen, M. Müller, …

    and at NIST or DXC2012: B. Cross, S. Fess, T. Jach, A. Schwartz
  - **objectives:** setting up a **work agenda**, dissemination to new members

International initiative on x-ray fundamental parameters

Objectives of the EXRS2012 event

- **Meeting of new expert groups in room MOE58** (max. 20 persons):
  - **Theory & codes – challenges: competent use and update of parameters**
    Monday 16.30 h
  - **New experimental determinations and methodology** **Tuesday 15.40 h**
  - **Integration of new experimental as well as theoretical parameters into critically evaluated compilations** **Thursday 12.30 h**
  - **Establishment of a common data base accessible to the public** **Fr. 10:00 h**
  - **Project management and fund raising** **Friday 10.45 h**