Report of 34th IUVSTA Workshop on "XPS: From Spectra to Results – Towards an Expert System"

Hotel de l'Univers, St. Malo, France, April 21-26, 2002

J. E. Castle and C. J. Powell (co-chairs)

X-ray photoelectron spectroscopy (XPS) is a commonly used tool for surface analysis in many scientific and technological applications. While XPS is a powerful tool as now applied, the Workshop organizers believed that the technique would be of much greater value if an expert system could be developed to guide users in the design of experiments and the interpretation of results.

The St. Malo Workshop was attended by 63 XPS experts from 16 countries (Australia, Austria, Belgium, Canada, Denmark, France, Germany, Hungary, Italy, Japan, New Zealand, Poland, Slovenia, Sweden, UK, and USA). The program was developed with the assistance of an International Program Committee consisting of J. E. Castle (UK), J. T. Grant (USA), L. Kover (Hungary), E. Ollivier (France), C. J. Powell (USA), M. P. Seah (UK), and K. Yoshihara (Japan). The local chairman was Dr. J.-P. Langeron (France), and the local committee consisted of J.-P. Langeron, B. Dallery, and V. Pfohl. Administrative arrangements were capably provided by the French Vacuum Society.

The Workshop program is attached. The program for the first day consisted of a plenary session. Prof. K. Ahmad (University of Surrey, UK) spoke on knowledge management, with emphasis on best practice and the possibility of new discoveries. He considered expert systems as a precursor to knowledge management, machine learning programs (neural nets), and information retrieval systems that could provide access to textual data (as found in journals and handbooks) and databases of materials-property data that are available on the internet. Dr. E. Ollivier (European Aeronautic Defence and Space Company, France) described possible experimental objectives for an expert system. The third plenary speaker, Prof. Castle, proposed the use of “wizards” that could be invoked in a future XPS expert system to provide enhanced guidance to an analyst in the design of an experiment (for a specified type of material and objective) and more powerful interpretive tools.

Workshop attendees were asked to participate in extended discussions with one of the following six Groups:

A. Instrument and Specimen Characterization (Leader: Dr. M. P. Seah, UK National Physical Laboratory)

B. Experimental Objectives (Leaders: Dr. E. Ollivier and Dr. S. W. Gaarenstroom, General Motors Research and Development Center, USA)

C. Wide-Scan Interpretation - Trial Composition and Structure (Leader: Prof. Castle)

D. Protocols for Narrow Scans, Instrument Setup, and Data Acquisition (Leader: Prof. P. M. A. Sherwood, Kansas State University, USA)

E. Reduction of Narrow-Scan Data - Chemical State and Morphology Analysis (Leader: Prof. W. S. M. Werner, Technical University of Vienna, Austria)

F. Reduction of Narrow-Scan Data - Quantification (Leader: Dr. C. J. Powell, National Institute of Standards and Technology, USA)

The leaders of each Group gave introductory presentations in the plenary session to outline the proposed work of their Groups. After this oral session, there was a poster session at which 32 poster papers were presented. These poster papers included descriptions and demonstrations of available software and databases for XPS.

On the following days, the six Groups met separately to discuss procedures, algorithms and data that might be incorporated into a future XPS expert system. The attendees were asked to think broadly about the structure and function of such an expert system, and not to consider details or issues associated with implementation. There was an intermediate plenary session at which preliminary conclusions and issues from each Group were presented and discussed and a final session at which the work of each Group was summarized.

The Workshop was very successful. The participants were enthusiastic about their tasks, and each Group produced many recommendations. There was a good mix of experience and expertise, and a vast amount of information was contributed.

It is planned to publish a summary of the Workshop (as was done for an earlier IUVSTA Workshop on XPS in 1999) so that other scientists can access the information (and comment on it). It is also expected that the details of the recommendations will be made available on one or more web sites. While it was thought possible that manufacturers of XPS instruments might be motivated (because of the Workshop and the resulting availability of consensus recommendations from XPS experts) to develop elements of the proposed expert system in their software, it was also believed that individual software developers might develop software products for more limited purposes. In addition, the Workshop recommendations are expected to become a valuable source of “best practices” in XPS. This material will be a valuable educational resource for both novice as well as experienced users.

XPS: From Spectra to Results – Towards an Expert System

St. Malo, France, April 21-26, 2002

Workshop Program

Sunday April 21: Arrival at Hôtel de l'Univers, Dinner at 8:00 pm

Monday April 22: Main Room, Hôtel de l'Univers (plenary session)

Chair: C. J. Powell

8.30 am	*J.-P. Langeron*, Welcome, information on logistics
8.40 am	*M.-G. Barthes*, Welcome to Workshop
8.45 am	*C. J. Powell*, "Introduction to Workshop, Information on Relevant ISO Standards, and Summary of Suggestions sent by Attendees"
9.00 am	*K. Ahmad*, "Knowledge Management: The Preservation of Best Practice and the Discovery of Things New"
9.40 am	Discussion
10.00 am	Coffee Break
10.30 am	*E. Ollivier*, "Experimental Objectives for an XPS Expert System, and Planned Work of Group B"
11.10 am	Discussion
11.30 am	*J. E. Castle*, "A Wizard Source of Expertise in XPS, and Planned Work of Group C"
12.10 pm	Discussion
12.45 pm	Lunch

Chair: J. E. Castle

2.00 pm	*M. P. Seah*, "Planned Work of Group A"
2.20 pm	Discussion
2.30 pm	*P. M. A. Sherwood*, "Planned Work of Group D"
2.50 pm	Discussion
3.00 pm	*W. S. M. Werner*, "Planned Work of Group E"
3.20 pm	Discussion
3.30 pm	*C. J. Powell*, "Planned Work of Group F"
3.50 pm	Discussion
4.00 pm	Coffee Break

Chair: J. T. Grant

4.20 pm	Short presentations on current capabilities of XPS software and databases (*Robinson, Green, Maehl, Vegh, Crist, Jo, Tougaard, Werner, Mohai, Hesse, Powell*)
6.00 pm	Poster session and demonstrations of software and databases

(1) *K. Robinson*, "Avantage Data System – An Overview"
(2) *M. Green, P. Grossman, and J. Westermann*, " EIS: Software for Electron and Ion Spectroscopy"
(3) *J. Westermann, M. Sander, D. Funnemann, and S. Pringle*, "High Count-Rate Detectors in High-Resolution Electron Spectrometers"
(4) *P. Ruffieux, P. Schwaller, O. Groening, L. Schlapbach, P. Groening, J. Westermann, Q. C. Herd, and D. Funnemann*, "Experimental

Determination of the Transmission Factor for the Omicron EA 125 Electron Energy Analyser"

(5) *S. Maehl*, "Architecture and Functionality of SpecsLab: The Data Acquisition and Processing Software from SPECS"

(6) *J. Vegh*, "XPS4XPS: A Possible Implementation of an Expert System for XPS/AES"

(7) *B. V. Crist*, "The "SpecMaster" XPS Spectral Database System and Spectral Data Processor (SDP) v3.0"

(8) *M. Jo*, "Program for Background Optimization"

(9) *S. Tougaard*, "XPS-Quantitation: QUASES Algorithms I, II, III"

(10) *S. Tougaard*, "XPS-Quantitation: QUASES Algorithms IV, V"

(11) *W. Smekal, W. S. M. Werner, and C. J. Powell*, "Simulation of Electron Spectra for Surface Analysis (SESSA)"

(12) *W. S. M. Werner*, "Partial Intensity Analysis: A Universal Method for Inelastic Background Analysis of Electron Spectra"

(13) *A. Schnellbuegel and R. Anton*, "Quantitative Analysis of X-ray Photoelectron Spectra of Rare Earth Fluorides"

(14) *M. Mohai and I. Bertoti*, "Calculation of Layer Thickness on Curved Surfaces by XPS MultiQuant"

(15) *R. Hesse, T. Chasse, and R. Szargan*, "UNIFIT 2002 – Spectrum Processing and Analysis Software of Core Level Photoelectron Spectra"

(16) *C. J. Powell and A. Jablonski*, "NIST Data Resources for Surface Analysis by AES and XPS"

(17) *A. Jablonski*, "Software for Determination of the IMFP from Elastic Peak Intensity"

(18) *D. Briggs,* "The XPS of Polymers CD-ROM Database from SurfaceSpectra LTD"

(19) *G. Speranza, R. Canteri, and M. Anderle*, "Some Considerations About the Analysis of Polymeric Materials by XPS"

(20) *N. Cioffi and L. Sabbatini*, "Simple Equations for Curve-Fit Data Treatment to Obtain Quantitative Information on Polymer Structure"

(21) *D. R. Baer*, "Practical Aspects of Surface Charge Control and Charge Correction in XPS: Current Art and Understanding and a Proposed ISO Standard on Reporting of Methods Used for Charge Control and Charge Correction (ISO 19318)"

(22) *C. E. Bryson*, "Expert System for XPS – Surface Potential Control"

(23) *S. Oswald, R. Reiche, and S. Baunack*, "Application of Factor Analysis in Electron Spectroscopy"

(24) *J. C. C. Day and R. K. Wild*, "Towards an Expert System – A Practical Approach"

(25) *S. Tanuma*, "The Use of Experimentally Determined Relative Sensitivity Factors for Quantitative Analysis by XPS"

(26) *J. Toth*, "Algorithm for Automatic Chemical State Determination by XPS"

(27) *L. Kover*, "Deriving Chemical Information from X-ray Induced

Electron Spectra"
(28) *M. Kurth and P. C. J. Graat*, "Quantitative Analysis of the Plasmon Loss Intensities in XPS Spectra of Magnesium"
(29) *L. Vanzetti, E. Iacob, M. Barozzi, D. Giubertoni, M. Bersani, and M. Anderle*, "X-ray Photoelectron Spectroscopy of Nitrided Silicon-Silicon Oxide Interface"
(30) *E. Ollivier*, "Theme B: Experimental Objectives for an XPS Expert System"
(31) *C. Blomfield, A. Roberts, and S. Hutton*, "Vision Data System – An Overview"
(32) *A. Tanaka*, "Practical Transmission Correction for XPS Analyzers with a Self-Consistent Transmission Function"

7.00 pm Adjourn
8.00 pm Dinner

Tuesday April 23

8.30 am Separate Meetings of Groups A to F (different locations)
10.30 am Coffee Break
11.00 am Separate Meetings of Groups A to F (different locations)
12.45 pm Lunch
2.00 pm Separate Meetings of Groups A to F (different locations)
3.45 pm Coffee Break
4.15 pm Separate Meetings of Groups A to F (different locations)
5.30 pm Continuation of poster session and demonstrations of software and databases
6.30 pm Adjourn
7.00 pm Reception by the Lord Mayor of St. Malo
8.30 pm Dinner

Wednesday April 24: Main Room, Hôtel de l'Univers (plenary session)

Chair: L. Kover

8.30 am *M. P. Seah*, Final Report of Group A and Discussion
9.10 am *E. Ollivier*, Final Report of Group B and Discussion
9.50 am Status Reports by Leaders of Groups C, D, E and F and Discussion
10.30 am Coffee Break
11.00 am Separate Meetings of Groups C to F (different locations)
12.45 pm Lunch
2.30 pm Excursion to St. Malo (until 5.30 pm)
7.30 pm Dinner at "La Porte Saint-Pierre"

Thursday April 25: Main Room, Hôtel de l'Univers (plenary session)

Chair: E. Ollivier

8.30 am Status Reports by Leaders of Groups C, D, E and F and Discussion
9.50 am Separate Meetings of Groups C to F (different locations)
10.45 am Coffee Break
11.15 am Separate Meetings of Groups C to F (different locations)

12.45 pm	Lunch
2.00 pm	Separate Meetings of Groups C to F (different locations)
3.45 pm	Coffee Break
4.15 pm	Separate Meetings of Groups C to F (different locations)
6.30 pm	Adjourn
8:00 pm	Dinner

Friday April 26: Main Room, Hôtel de l'Univers (plenary session)

Chair: M. P. Seah

8.30 am	*J. E. Castle*, Final Report of Group C and Discussion
9.10 am	*P. M. A. Sherwood*, Final Report of Group D and Discussion
9.50 am	*W. S. M. Werner*, Final Report of Group E and Discussion
10.30 am	Coffee Break
10.50 am	*C. J. Powell*, Final Report of Group F and Discussion
12.00 pm	Adjourn