



Surface Analysis Forum Newsletter No. 18

Spring 1995



Contents



Physico-Chemical Parameters from Surface Analysis

Report on the January meeting at the University of Surrey. The main articles are stored as gif files because they contain equations which some browsers might otherwise have difficulty in displaying. Also included are reports on the group sessions including:-

Standardisation in Instrument Specification

The Practical use of Chemical Shifts in XPS/AES

The Future of Data Processing



News in Brief

ESCA users archive, job required, surface science news group



Report of ISO/TC 201 Meeting in Golden, Colorado

Report on the second full ISO meeting on Surface Chemical Analysis



Report on the 41st National Symposium of the American Vacuum Society



Meeting Report

Physico-Chemical Parameters from Surface Analysis

University of Surrey

Thursday 5th January 1995

These articles are stored as gif files as they contain equations that some browsers might otherwise have difficulty in displaying.

(Note:- I lost the gifs when i moved servers, sorry.)

Page 1. A talk by Prof. Jim Matthew (University of York) on the development of our knowledge and appreciation of chemical shifts in XPS and AES. (56k)

Page 2. Continued from page 1. (69k)

Page 3. A talk by Martin Seah (NPL/DTI) on the use of surface analysis to provide well known physical parameters such as refractive index, surface energy and work of fracture. Also a talk by Jim Castle (University of Surrey) on getting as much as possible out of XPS results and means of interpretation which can be used by nonspecialists. (63k)

Page 4. Continued from Page 3, also a talk by Peter Weightman (IRC, Liverpool) on the calculation of a new scale of electronegativity. (74k)

Page 5. Continued from page 4. (37k)



The afternoon session was dedicated to workshops.

Standardisation in Instrument Specification

Leader Bob Wild (IAC, Bristol)

Rapporteur Alison Taylor (University of Surrey)

Bob outlined the operation of two ISO TC 201 & BSI C1160 standards committees. Members of the UK Surface Analysis Forum are closely involved with these committees and the existence of the Group has helped in formulating a coherent UK response to various proposed standards. The aim of the workshop was to gather points of view from both manufacturers and customers regarding what they require from instrument standardisation. John Watts is currently collating data from manufacturers.

The potential merits of standardisation were recognised by everyone although, in the past, manufacturers had presented performance indicators derived from nonstandard methods. Deciding which parameters should be presented to customers was a potential problem. Outline specifications for discussion were thought too detailed and there were cost implications in terms of time in test. It was therefore agreed that a list of key parameters should be produced with a procedure for measuring them. The intensity and energy resolution on the Ag3d peak were accepted parameters but S/N and S/B were still being debated. Any list of parameters could be added to subsequently but the important aspect is that they are obtained using a standard procedure.

Actions from the meeting were 1) John Watts to collate manufacturers specification sheets and produce a summary, 2) John and Bob will begin to draft standard procedures

for obtaining key parameters for discussion at the next BSI meeting in April 1995.



The Practical use of Chemical Shifts in XPS/AES

Leader & Raporteur Len Hazell

This workshop began with a review of the theory and how soon it will be of direct practical value in analysis. The combination of work in Groups at Liverpool and York is in the vanguard of calculating chemical shifts. The ultimate aim is to be able to calculate the peak position of a given molecular structure and vice versa. However there are still some unknowns and application to complex systems is unlikely for some years.

There was an extended discussion of the practical problems in measurement of chemical shifts. This ranged over 1) the problems of sample charging, particularly with monochromators, 2) the need for background subtraction and curve resolving, 3) whether knowledge of the spectrometer performance could be used to assess the peak widths for curve resolving (answer NO!) and 4) the use of combined XPS/AES shifts in the form of the Auger parameter. The conclusions were that, as analysts, we were doing the right sorts of things and nothing fundamentally new had been introduced for many years now. There was an appeal for a single button fully compensating charge neutralisation system for use with the greatly improved specification monochromators now available.

Most elements possessed useful chemical shifts but interpretation depended on published literature, home grown reference compounds (mostly not easy to generate) and databases. Unfortunately, the precision of data in available databases is variable because the original data was not acquired under accredited conditions. This may be an area that will have to be readdressed after accreditation status has been achieved by a larger number of Groups.

The benefit of the workshop was that members had gained a better appreciation of the meaning, value and necessary acquisition strategy for measuring chemical shifts but it was disappointing to realise how much more needs to be done before theory can help us identify compounds on surfaces.



The Future of Data Processing

Leader Albert Carley
Raporteur Martin Seah

This workshop was carefully structured to consider the overall purpose of data systems, the problems of upgrades as equipments ages, essential developments for future data systems and possible directions for the future.

Data systems are used for both acquisition and data processing. In most cases the analysis time could be used more effectively. Aging data systems were difficult to support and need to be replaced eventually. There was now a healthy competitive environment with the availability of third party systems.

Users would like to see increased intelligence and automation to (1) relieve expert staff of

slow repetitive tasks and (2) to ensure that all analysts could work to the best practice standard of the experts users. Increased automation, either to a user's recipe or an approved standard, would be welcomed. Data integrity had to be maintained and the recipe documented with the data file. The validation of software routines become more and more important as the complexity increases. Aspects of peak deconvolution, reconstruction of depth profiles from angle-resolved data, maximum entropy processing, error analysis and quantification were discussed.

The above list of items showed that data processing software needed continual upgrading whereas the acquisition software only needed periodic revision. One useful way of allowing upgrades was to adopt a modular approach where user defined activities can be built around a general platform such as MATLAB. Tracking of version numbers and validation is essential however.

Five main concepts for processing software featured repeatedly throughout the discussion, Automation, Flexibility, Modularity, Upgradability and Validation. Standardisation, used effectively to generate best practice recommendations and checking routines could promote this; used ineffectively, it could become a straightjacket.

News in Brief

ESCA Users Archive

Those of you who still have as yet not sent any papers to the archive should know that the archive is about to be computerised. It will be linked to an existing Surface Analysis Archive which dates back to the early 1970's! So if you wish to be included in the New ESCA Users archive send your papers a.s.a.p
S.J.Harris

Job Required

Dr A.Zagorenko has written to me concerning a possible position in this country. Anyone who has a position available at present and would be interested in contacting Dr Zagorenko, please do so via the address below or contact me for further details.

Dr A.Zagorenko
27, rue de Maurepas
92500 Rueil-Malmaison
France
Tele 33-1-47528035
Fax 33- 1 46527057
Email zagorenko@irvaxl.ifp.fr

Surface Science News Group (For Email Users Only)

A newsgroup has been set up in Canada which will discuss problems, advertise jobs and meetings. The news group is for Email users only (sorry Martin), and the mechanism by which you can join the group is shown on the opposite page.
S.J.Harris

Report of ISO/TC 201 Meeting in Golden, Colorado

20-22 October 1994

This is a brief report of the second full ISO meeting on Surface Chemical Analysis. Twelve members of the BSI/CII/60 attended in various capacities. They were Martin Seah, Dave Sykes, Albert Carley, John Watts, Bob Wild, Suganta Biswas, Bob Bulpett, Alan Carrick, Peter Coxon, Steve Harris, Mike Wells and Alan Wirth.

This meeting was the first to occur after the various sub-committees and Working Groups had been constituted and discussions about real standards were starting. I include at the bottom of this report a table showing the various sub-committees and Working Groups with their respective Chairmen, Secretaries and Covenors. Some Sub Committees are further advanced than others. SC3 on Data Management and Treatment already have the VAMAS Data Transfer Format as a New Work Item that should become a standard in the not too distant future. Others have tried to introduce standards quickly but have come up against problems. However most Working Groups spent the time at Denver outlining frame plans for the production of standards. For example in my own Sub Committee SC7 on XPS John Watts is leading the Working Group on Instrument Specification. It has been decided that the first step must be to identify how manufacturers currently specify their instruments before moving on to get some conformity so that eventually all users will be able to compare specifications knowing that each manufacturer specifies in the same way. Bob Bradley is leading SC3 WG3 on Algorithms for Data Treatment and here groups have identified areas for algorithms that will be recommended, such as background subtraction, smoothing etc.

It was intended that all the work was discussed sequentially so that everyone had the opportunity to discuss all topics and in the main this was successful with only a few breakaway groups. The UK view was ably put by all the delegates but I would like to single out Mark Dowsett who made a considerable impact in the areas of Depth Profiling and SIMS. Discussions were friendly and a consensus was invariably reached on most issues.

R. K. Wild

41st National Symposium of the American Vacuum Society

This year the meetings of the ISO committee TC/201 on Surface Chemical Analysis met in association with the 41st National symposium of the American Vacuum Society in Denver last October. Not many of your colleagues took the opportunity to attend this conference and so your committee thought it would be useful for me to provide a brief tour of the meeting. The registration is about 160 pounds for members and good hotel rooms were available down to 36 pounds per night so the costs for the whole meeting could be around 850 pounds (quite comparable to a similar length meeting in Europe).

One advantage of the AVS meetings is that they are large. About 1400 papers were presented with a large number of very high quality pieces of work. These are easily grouped into eleven parallel sessions covering applied surface science, thin films, basic surface science, electronic materials, biomaterials, nanoscale science and technology, vacuum technology, plasma science, vacuum metallurgy etc. In these sessions there are

three invited speakers per day so arranged that their times do not, in general, clash. This means you can easily get up to speed in, say diamond-like films, biosensor interfaces and nanomechanics all on the same afternoon. The areas covered by the Applied Surface Science Division were "Imaging and Small Area Analysis", "Data Processing and Reference Methods", "Surface Chemistry and Contamination", "Electrochemistry and Liquid/Solid Interfaces", "Quantitative Analysis/ARXPS", "Depth Profiling" "Self-Assembled Monolayers", "Polymer/Organic Surfaces" and "Adhesion and Adhesive Bonding". Each topic had an invited lecture and some 8 to 10 oral contributions and further poster presentations. With this variety it may be difficult to make it to the equipment exhibition but lunchtime is scheduled as 2 hours and snacks are available amongst the 300 booths for vacuum, coating, surface analysis etc equipments.

Examples of some of the nice static SIMS work presented involved the clear ToF imaging of cyclic trimer PET crystallites on the PET surface and the lateral surface diffusion of PDMS on polymer surfaces. In XPS the Berkeley Advanced Light Source has achieved analysis of less than 30 microns at 0.1 eV energy resolution and MHz count rates. The design limit for spatial resolution is 25 nm. In AES we saw clear high resolution imaging of insulating diamond-like areas using EELS in the Fisons 310F system. Of potential interest to AES and perhaps more for electron beam lithography, early results were shown for a lithographed SEM with a design spot size of 38 Å. These use field or Schottky emitters. Coupled with the lithographed electron spectrometer shown last year and published in Journal of Vacuum Science and Technology (incidentally, if you cannot attend AVS most of the relevant papers, say 80%, are published in two large issues of JVSTA - the blue ones - in July-August of the following year). Lithography and micromachining is now a major topic area as a result of the development of a range of microactivators and microsensors for the motor and medical industries. A few old battles, which had been aired at QSA, concerning electron inelastic mean free paths and the development of ripples in sputter-depth profiling with oxygen ions, incremented forward. If one had already fully understood these problems, one could, for instance, learn instead about submicron magnetic islands, the engineering of atomically sharp STM tips, process-property relations in preparing nanocrystalline diamond films or the SIMS of covalently bonded peptides on fluoropolymers!

Although the AVS meeting has vacuum in the title, much of the nanoscale science and technology work, some of the tin films work and a little in most other areas no longer involve vacuum. AFM studies are often in liquid or the air. This shift in emphasis is one which will continue and today we find the Vacuum Technology Division is one of the few that does not have sessions throughout the week.

MP Seah
UK Surface Analysis Forum

Last updated 24 February, 2001

*Simon Morton
Advanced Light Source
Lawrence Berkeley Laboratory
Berkeley
CA 94720*

Comments or enquiries to S.Morton@uksaf.org