

Workshop Summary

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Introduction

The following section is a personal summary of the scientific presentations and vivid, detailed discussions on different aspects, methods and views of various problems in the field of electron scattering in solids. The intention is to highlight some of the main issues and results that are believed to be significant and that may influence future progress.

I. History of fundamental aspects

In his profound and comprehensive plenary lecture, Ritchie first gave a historical overview on the development of studies on scattering of charged particles in solids. The first theory on stopping power was created by Bohr in 1913, and the first full quantum theory of Bethe appeared in 1930. The dielectric formalism was developed by Fermi in 1940, and Lindhard elaborated his model on the dielectric response function of the electron gas in 1954. In 1957, Ritchie predicted the surface plasmon on the basis of the dielectric and hydrodynamic model, and in 1960 Powell found the first experimental evidence for surface plasmons in the case of Al and Mg.

Modelling the solid as a (nearly) free electron gas under high pressure proved to be successful. It turned out that the exchange correction in calculating the mean free path of electrons scattered inelastically in the solid (IMFP) was important below 1 keV electron energy. The orthogonality of surface and bulk excitation modes leads to a decrease of bulk electron energy-loss probability near the surface.

The dielectric representation of condensed-matter response as developed by Ritchie still provides a very important and useful framework for describing electron-scattering phenomena in solids.

II. Elastic electron scattering

Studies on the differential cross sections (DCSs) for elastic scattering of electrons were reviewed by Salvat and Jablonski.

The Static Field Approximation assumes purely electrostatic atomic potential and the target atom is regarded as a frozen distribution of electric charges. The interaction with the electron is purely electrostatic, and includes exchange, correlation and polarization. With this model systematic differences from experimental results occur at low and medium to large scattering angles.

The Optical Model potential accounts for atomic charge polarizability and contains an imaginary absorptive potential term. In applications, empirical parameters are used; no ab

initio calculations are performed. A molecular DCS is obtained as the sum of the atomic DCSs.

The optical potential model of Fujikawa is based on a non-local self-consistent theory. It works for small scattering angles as well, providing good agreement with experiments.

Jablonski compared the DCS results derived using two atomic models: the Thomas – Fermi - Dirac potential (based on a statistical model of the atom) and the relativistic Dirac – Hartree – Fock potential (from a self-consistent approach). DCSs from these models were compared with each other and with experimental DCSs. Large deviations between calculated DCSs from the two models occurred at low energies, small scattering angles and in the vicinity of deep minima in the DCSs. Comparing experiment to theory (50-3000 eV electron energy, noble gases, Hg) a good general agreement was observed at high energies but there were increasing deviations at lower energies and at small scattering angles (due the neglect of polarization effects) and near deep minima.

Dapor presented a method for obtaining DCSs in selected oxides, solving the Dirac equation for the central electrostatic field, using the relativistic partial wave expansion method (RPWEM). Analytical expressions involving a screening parameter were derived to approximate the results of the RPWEM. The method provides good general agreement with experiment; deviations are at small angles and at sharp minima. Limitations: 50 eV – 10 keV electron energy; atomic number up to $Z=30$.

High-energy-resolution experimental results (Varga et al.) were presented demonstrating the quasielastic scattering of electrons in polyethylene. Effects of H recoil in the REELS spectra in a backscattering experiment using primary electrons of a few keV energy were shown and proved for the first time.

A new version of a NIST database providing DCSs for elastic electron scattering was described by Powell.

III. Inelastic electron scattering in solids

Modeling of intrinsic and extrinsic excitations in the energy loss part of XPS and AES spectra was reviewed by Tougaard who compared fully quantum mechanical (QM) ab initio models (of limited practical applicability) and the semiclassical (SC) approaches based on the dielectric response theory. Good agreement is obtained between the QM and SC models for electron energies $E > 100$ eV.

Concerning the SC models, first the “two-step” model (assuming excitation described in sudden approximation and transport of photo- or Auger electrons in the solid) was mentioned. This model can be used for decoupling of effects due to extrinsic and intrinsic excitations. The model provides the “effective” intrinsic spectrum (which contains part of the interference). Second, the Yubero-Tougaard one-step model (describing energy loss of electrons in the frame of time-dependent perturbation calculations) accounts for surface and core hole effects, interferences between extrinsic and intrinsic excitations (negligible at energies higher than 1000 eV), and can be used for interpreting Auger peak shapes (due to the final state holes, a larger intrinsic contribution can be expected), describing the angular distribution of photoelectrons and separating the spectral contributions due to extrinsic and intrinsic excitations. Software based on the Yubero-Tougaard model has been developed that

requests the energy-loss function as an input. From various applications it has been found that 85 % of contributions due to surface excitation are of extrinsic nature but at low (grazing) emission angles the contribution from intrinsic excitations can rise to 60%.

A comment from Fujikawa: separation of the contributions from intrinsic and extrinsic excitations can depend on the theoretical framework!

Surface effects in electron spectroscopy were reviewed by Werner. Surface, intrinsic and bulk excitations are uncorrelated for medium energy (usually valid in XPS and AES) electrons (size of region where surface and intrinsic excitations occur is small compared to the elastic MFP). In many cases, the surface excitations and intrinsic contributions can be described by an integral parameter instead of depth-dependent IMFP. Through decomposition of spectra to contributions from surface, intrinsic and volume excitations, the coupling of surface and bulk excitations (Begrenzung) becomes directly observable.

The surface excitation probability in Reflection Electron Energy Loss Spectroscopy (REELS) experiments depends on the electron emission angle as well as on the scattering angle. A rectilinear part of the trajectory responsible for surface excitations can be assumed. Surface excitations can influence the angular distribution of the low energy Auger electrons. Analysis of many body effects in solid state electron spectra now becomes possible.

Kwei, using the dielectric response theory, described the memory effect of fast electrons moving parallel to a solid surface: the cross section for inelastic scattering depends on the energy of the electron before the previous interaction (due to the induced field).

Nagatomi, using the extended Landau theory, derived Surface Excitation parameters (SEPs) from analysis of the measured elastic peak and REELS spectra and comparison with Monte Carlo simulations (for Ni).

IV. Interference effects

The role of quantum interferences between surface-bulk, intrinsic-extrinsic excitations was reviewed by Fujikawa. First Hedin's Blue Electron theory (where the photoelectron is distinguished from others) was discussed. Then Fujikawa's quantum electron dynamical (QED) theory was described. This theory, using the Keldysh Green's function approach, accounts for relativistic many-body effects and photoelectrons are not distinguished from other electrons. The Inglesfield fluctuation potential is utilized to describe plasmons. The model leads to a rather good agreement with the experimental data. Interferences play an important role in describing the angular dependence of loss structures.

Quantum and classical (dielectric) theories of plasmon excitation in nanostructures (capillaries and wires) were compared by Gervasoni. There is an agreement between the two models for the average number of excitations. However, strong interferences were found along transverse trajectories (at some distances, characterized by a function of the diameter of the nanostructure, no plasmons are created), in the same way that were found in planar surfaces by the same authors.

IV. Inelastic Mean Free Paths

The present status of calculation of bulk IMFPs from experimental optical data was reviewed by Powell. Optical data available in the energy range 1 eV- 30 keV are used, following a consistency check with the help of internal sum rules. Algorithms with different technical approaches have been applied for calculating IMFPs. Selected examples from five different types of experimental measurements showed that the IMFPs from optical data were consistent with these measurements to generally about 10%. In one example, an interlaboratory comparison of SiO₂ overlayer thicknesses derived by XPS using IMFPs from optical data showed a consistency of ca 1% with layer thickness data obtained with other techniques. In another example involving comparisons of IMFPs derived from REELS spectra with IMFPs from the TPP-2M predictive formula, there was good agreement for Ti, TiC and TiN but poorer agreement for TiO₂ and for diamond and graphite. Concerning the application of the TPP-2M formula, recommended values are available now for an important parameter, the number of valence electrons per atom.

Tanuma presented IMFPs for 27 elemental solids in the energy region 50 eV – 5 keV that were derived from optical data using Penn's algorithm. He then made comparisons with IMFPs with IMFPs obtained using the Elastic Peak Electron spectroscopy (EPES) method and a Ni reference, for 12 elemental solids. Good agreement was found except below 100 eV electron energy (diffraction effects), within 7 % (except for Mo, Ga, and Zn). The TPP-2M formula gave a slightly worse agreement with experiment.

IMFPs determined by other methods were also presented. Sanz derived energy loss functions and IMFPs for amorphous carbon and boron, and their nitrides from quantitative analysis of REELS spectra using the Yubero-Tougaard model and parameterization in terms of Drude-Lindhard type oscillators, comparing the obtained data with those published earlier and with those predicted by the TPP-2M formula.

Akkerman used the dielectric function theory (self-consistent method) and the optical energy loss functions fitted by Drude type functions, to calculate electron IMFPs and stopping powers in alkali halides, metal oxides and organic compounds.

Based on the structural formula of a material alone, the Quantitative Structure-Property Relationship Method to obtain IMFPs was presented by Cumpson. The method can be applied in the case of materials where no information is available on band gap, density, etc. Special advantages of the method are expected for proteins and other biomaterials.

Surface effects on IMFPs were discussed by Gergely. IMFPs by EPES were shown for 5 elemental solids, often used as reference samples as well, in the energy region of 0.2 – 2 keV. Expressions were derived for IMFP ratios and Surface Excitation Parameters (SEPs). The SEP correction improved the agreement with Tanuma's data.

EPES-derived IMFPs in selected elements and polymers were presented by Lesiak who discussed corrections for surface excitations using different models. The deviations between corrected and uncorrected data were comparable to the deviations between different models: Werner's model was suggested as preferable.

Absolute measurements of elastic reflection coefficients (Si, SiO₂, Al, Cu), using a Retarding Field Analyzer were shown by Pavluch who also reported IMFPs with and without the SEP

correction. The IMFPs derived without the SEP correction agreed better with Tanuma's values, as expected.

Further challenges in IMFP determinations were pointed out in several contributions:

Menyhárd discussed IMFPs for ultrathin oxide films obtained from EPES and REELS studies during ion beam depth profiling. Excellent agreement is found between experiments but good or poor (e. g. HfO_2) agreement is found with calculated IMFPs. Is the concept of an Effective IMFP the solution ?

IMFP values for GaAs(100)-c(4x4) in the energy range 10-40 eV, derived from photoelectron spectra (overlayer method using a GaAlAs delta layer as a "substrate", normal Al 2p photoemission) excited by tunable synchrotron radiation, were presented by Jiricek. Can the large maximum (as a function of electron energy) occurring in the IMFP curve at about 30 eV be attributed to the effect of the unoccupied density of electronic states ?

IMFP ratios as a function of energy, determined by XPS, using characteristic X-rays of different energies for excitation, were compared with IMFPs derived using the EPES method by Tóth showing the applicability and limitations of this approach.

V. Characteristic distributions

The advantages and applications of a new Monte Carlo (MC) simulation algorithm, developed to describe the angular and energy distributions of backscattered electrons after elastic and inelastic scattering events, was demonstrated by Jablonski. This algorithm was used to determine the lateral distribution of Auger emission and for calculations of Auger linescans across an edge and of the analysis area.

Zemek reported on the experimental determination of the XPS Emission Depth Distribution Function for an iron oxide film, using opposite-side X-ray excitation and measuring the intensity of the O1s photopeak as a function of overlayer thickness. Good agreement with theory was obtained.

Effective Energy Loss Functions (EELF) derived from REELS were presented by Zhang who modeled the EELF by linear combination of the theoretical DIIMFP (Differential Inverse Inelastic Mean Free Path) for surface and bulk excitations.

A novel, invariant embedding technique for describing electron backscattering distributions was reported by Glazov. The distribution of backscattered electrons, as a function of the numbers of elastic or inelastic collisions, incident or emission angles, and path length within the solid, is provided quickly and without numerical simulation. Inclusion of an extra variable does not lead to a drastic increase in computing time and effort.

VI. Databases and software describing electron transport in solids

Databases available from NIST for electron spectroscopy were reviewed and demonstrated by Powell, including the XPS, the Electron Elastic-Scattering Cross-Section, the Electron Inelastic-Mean-Free-Path, the Electron Effective-Attenuation-Length Databases.

New software for determining electron IMFPs using the EPES method, EPESWIN was introduced and demonstrated by Jablonski.

Tougaard demonstrated the QUASES software family – based on semiclassical dielectric models and the Landau formalism. The software packages provide tools for quantitative modeling of XPS, Auger, Angle-Resolved XPS, REELS spectra, effects of extrinsic excitations in XPS and AES spectra, and effects of intrinsic (core-hole) and surface excitations.

A planned new NIST Database for the Simulation of Electron Spectra for Surface Analysis (SESSA) was described and demonstrated by Werner and Smekal. SESSA contains comprehensive databases (cross sections, lineshapes, transport parameters, fully traceable) and a small expert system. Simulation of XPS and Auger spectra of layered samples is possible, thus allowing the determination of composition and layer thickness by comparing measured and simulated spectra. Further applications: simulations of Total Reflection XPS, Auger and Photoelectron Coincidence, REELS, and EPES spectra.

Végh demonstrated his wxEWA program that uses pseudocomponents linked to main components for improving the performance and accuracy of spectrum evaluation.

Software for simulation of Energy Dispersive X-ray spectra induced by an electron beam (in a Scanning Electron Microscope, SEM) and emitted from samples with rough surfaces was developed and demonstrated by Gauvin. The program calculates absolute intensities of characteristic and bremsstrahlung spectra, the accuracy is about 20 % for primary electron energies above 10 keV.

VII. Novel techniques

Goto reported on absolute intensity and energy measurements in AES, work function measurements with a special PhotoEmission Electron Microscope, and on determining analyzer transmission with a new method.

A model describing electron–solid interactions at very low energies (<50 eV), and electron transport in dielectrics in the presence of an electric field was presented by Akkerman. He also showed the relationship of this approach to models valid for higher energies.

The use of photoelectron diffraction for distinguishing two coexistent non-equivalent orientations of complicated molecules (C-60) adsorbed on surfaces was demonstrated by Cepek, who applied synchrotron radiation and single-scattering-cluster modelling.

Methods developed for removing contributions from multiple electron scattering in Electron Momentum Spectroscopy of solids from coincidence experiments were reviewed by Vos. Modeling of electron energy-loss and elastic scattering makes it possible to recover information on the electronic structure of the material under investigation, as demonstrated for polycrystalline (Al) and single crystal (Cu) metals.

Electron Pair Spectroscopy was introduced by Williams who discussed spin-dependent scattering dynamics, spin-resolved electronic structure, and spin-polarized (e,2e) experiments (25 eV incident electron energy). Spin-orbit coupling effects were demonstrated in inelastic scattering of low energy electrons from W(110).

VIII. Image Contrast

Recent developments in the field of Low Voltage (LV) and Very Low Voltage (VLV) SEM were reviewed by El Gomati. The high lateral resolution (a few nm) attained gives possibilities for 2D profiling. Advantages : surface sensitivity, high SE yield, Z contrast, primary electron energy $E_p = 1-3000$ eV. Applications: studying ULSI materials, distribution between n-type and p-type dopants. The role of sample conditions and vacuum environment (cleaning) is important. Problems: lack of clear models for interpreting image contrasts, repeatability, dependence on SEM, primary energy. The Low energy Scanning Analytical Microscope combines Auger Electron Microscopy with VLVSEM and can be used for imaging electronic structure of surfaces with nanostructures. As an example, the appearance of SE contrast of doped semiconductors in LVSEM as a consequence of formation of ohmic and rectifying contacts by thin metallic surface layers was demonstrated.

The problems of MC simulation of SEM images of complex structures were discussed by Ding, including SE yields, structure of specimens and varying mean free paths. His new parallel MC simulation program, using ray tracing and corrected trajectory lengths across different zones, simulates SEM images for inhomogeneous samples with complex structures.

IX. Further applications of electron transport phenomena in solids

A new method for quantitative X-ray microanalysis of real materials using MC simulation was developed by Gauvin, who described quantitative microanalysis of spherical inclusions embedded in a matrix. The method is also applicable for the analysis of multilayers.

A method for determining the lifetimes of quasiparticles (elementary excitations) and for estimating charge and energy transfer at surfaces was discussed in the paper of Echenique (presented by Gervasoni). Results on electron and hole dynamics for bulk and surface states were provided.

MC simulations of low energy elastic reflection of electrons by solids were presented by Stary who compared the results with EPES measurements (yield ratios) in the 0.2 – 2 keV electron energy range for C, Al, Cu, Ag, Au, Si and SiO₂. Concerning the energy dependence, a good agreement is obtained for light elements and this is improved by including correction for surface energy losses.

Gruzza reported on the Multi-Mode EPES method to vary the primary electron energy for changing the depth of analysis of the surface region. The MSEP (Monte Carlo Simulation of Elastic Peak) software was developed for interpreting the experimental results. Stacking-layer models are available for simpler cases.

Surface losses at large distances from metal surfaces were discussed by Tőkési, who derived the surface loss function within the specular reflection model and the Time Dependent Density Functional Theory (Local Density Approximation, Random Phase Approximation). The calculations separate p-hole and plasmon excitations.

42nd IUVESTA Workshop *Electron Scattering in Solids: from Fundamental Concepts to Practical Applications (ESS'04)*

July 4-8 2004, Debrecen

Co-sponsored by the Applied Surface Science and the Surface Science Division of IUVESTA

I. Brief Scientific Report

Knowledge of electron scattering processes in solids is needed for the surface analysis techniques of Auger-electron spectroscopy (AES) and X-ray photoelectron spectroscopy (XPS), the bulk and thin-film analysis technique of electron-probe microanalysis (EPMA) and the surface-characterization technique of scanning electron microscopy (SEM).

The Workshop, similarly to the very successful previous IUVESTA Workshops on Auger Electron Spectroscopy: From Physics to Data (Saint Pierre de Chartreuse, France, 1995, reported in Surf. Interface Anal. **26**(1998)72); on X-ray Photoelectron Spectroscopy : From Physics to Data (Hortobágy, Hungary, 1999, reported in Surf. Interface Anal. **29**(2000)671) and on XPS: From Spectra to Results-Towards an Expert System (Saint Malo, France, 2002, reported in Surf. Interface Anal. **36**(2004)225) under IUVESTA sponsorship, brought together experts in the field of Electron Scattering in Solids. There were two related International Workshops held in recent years on the Electron Inelastic Mean Free Paths (Budapest, Hungary, 2000, and Prague, Czech Republic, 2002).

The organization of the 2004 Workshop was motivated by *(i)* the recent progress in experimental methods and theoretical models studying electron-solid interactions, *(ii)* the significance of knowledge of elastic and inelastic electron-scattering processes in solids for quantitative applications of electron spectroscopies. The aims of the Workshop were *(i)* to review the present status and level of understanding in the field of electron scattering processes in solids, *(ii)* to identify issues of key importance (*hot topics*) in the light of most recent scientific results, and *(iii)* to stimulate discussions leading to a deeper understanding and to new solutions for the existing problems.

The scientific field and scope of the Workshop falls within the area of activity of the Surface Science and the Applied Surface Science Divisions of IUVESTA. Attendance at the Workshop of key experts was ensured in the first instance by invitation. Many of the best and most active researchers of the field participated in the meeting. The 50 participants of the ESS'04 Workshop represented 20 countries (including 16 member countries of IUVESTA) of Asia, Australia, Europa, and North and South America.

The scientific program of the meeting was developed by the Scientific and Program Committee, co-chaired by L. Kövér (Hungary) and C. J. Powell (USA) and including J. T. Grant (USA), A. Jablonski (Poland), M. Menyhárd (Hungary), M. P. Seah (UK), S. Tanuma (Japan), S. Tougaard (Denmark) and W. Werner (Austria). The Local Organizing Committee, with L. Kövér (Chairman), E. Bene, Z. Berényi, I. Cserny and J. Végh (members) was responsible for most of the local matters of organization and for ensuring appropriate conditions for the meeting. Registration, contracts for accommodation, meals and transportation were arranged by the Roland Eötvös Physical Society (Budapest), represented by Mrs. Margó Nagy, Acting Secretary.

The structure of the scientific program based on sessions each of 1,5 h duration, including 9 Invited Reviews on specific fields, 35 contributed presentations on 'hot topics' and 7 presentations on software development and databases. In each session, enough time was ensured for extended and intense scientific debates and discussions among the experts present. The sessions were moderated by selected experts of the particular topics. At the end of the meeting, a closing summary of the technical content of the Workshop was provided. The scientific program for the Workshop and the list of the participants are attached. Although no proceedings of the Workshop will be published, a detailed Report including brief summaries of the contributions and the discussions is planned to be submitted for publication, as for the previous Workshops mentioned earlier.

The venue of the meeting was the four star Aquaticum Thermal and Wellness Hotel, an integrated part of the unique spa, health service and leisure complex situated in the heart of the idyllic Debrecen Great Forest, providing full comfort and a nice environment for the delegates and ensuring a quiet place for the Workshop. A guided city tour in Debrecen, introducing its historical sites, completed the very dense technical program.

II. Financial Statement

Here it is certified that the financial support of 10.000.- CHF provided by the IUVSTA for the *IUVSTA Workshop on Electron Scattering in Solids – From Fundamental Concepts to Practical Applications*, was fully used to cover fixed costs, namely the cost of the invited contributors, including the 9 Invited Reviewers, 6 Invited (oral) Contributors and one Session Moderator (moderating two sessions).

Debrecen, 2004. August 11.

László Kövér and Cedric J. Powell
Co-chairmen, Scientific and Program Committee

IUVSTA Workshop on Electron Scattering in Solids

July 4-8 (Sunday – Thursday), Debrecen

Program

i. **Sunday, July 4**

17:00 – 19:00 Registration

19:00 – 21:00 Reception (Thermal & Wellness Hotel)

ii. **Monday, July 5**

8:00 – 10:00 Registration

9:00 – 9:30 Opening

H.-J. Mathieu, Chairman, Applied Surface Science Division, IUVSTA

J. T. Grant, Chairman, Publications Committee, IUVSTA

D. Berényi, Hungarian Academy of Sciences

R. G. Lovas, Director, Institute of Nuclear Research of the Hungarian Academy of Sciences

C. J. Powell, Co-Chairman, International Scientific and Program Committee

L. Kövér, Co-Chairman, ISPC, Chairman, Local Organizing Committee

9:30 – 10:30 I. Plenary Session

Moderator: **C. J. Powell**

9:30 – 10:15 **R.H. Ritchie**: Elastic and Inelastic Scattering of Electrons in Solids and near Surfaces – *Plenary Lecture*

10:15 – 10:30 Discussion

10:30 – 11:00 *Break*

11:00 – 12:20 II. Elastic Scattering of Electrons by Atoms and Solids 1.

(Atomic models and calculations of differential cross sections for elastic scattering)

Moderator: **A. Jablonski**

11:00 – 11:35 **F. Salvat**: Calculation of Differential Cross Sections for Elastic Scattering of Electrons by Atoms and Solids – *Invited Review*

11:35 – 11:50 **T. Fujikawa**, H. Arai, H. Shinotsuka: Theory of Atomic Optical Potential in Solids

11:50 – 12:20 *General Discussion*

12:20 – 13:50 *Lunch*

13:50 – 15:30 III. Elastic Scattering of Electrons by Atoms and Solids 2.

(Comparison of calculated and measured differential cross sections for elastic scattering)

Moderator: **J. F. Williams**

13:50 – 14:25 **A. Jablonski**: Comparison of Differential Cross Sections for Elastic Scattering of Electrons: Calculations and Measurements – *Invited Review*

14:25 – 14:40 **M. Dapor:** Calculation of the Elastic Scattering Cross Sections of Electrons in Selected Oxides

14:40 – 14:55 D. Varga, Z. Berényi, K. Tőkési, **J. Tóth**, L. Kövér: Energy Distribution of Electron Beams Backscattered from Solids: Energy Shift and Broadening due to Atomic Recoil

14:55 – 15:30 General Discussion

15:30 – 16.00 *Break*

17:00 – 19:00 IV. Software Demonstration & Poster Session

Moderator: **J.T. Grant**

16:00 – 17:00 Introduction to the Software Demonstration (*Brief presentations, max. 10 min*)

C. J. Powell: NIST Databases for Applications in Electron Spectroscopy

A. Jablonski: Software EPESWIN for Determination of the IMFP from Elastic Peak Intensity

S. Tougaard: Software for Quantitative Analysis of Electron Spectra

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

J. Végh: Using Pseudo Components for Improving Spectrum Evaluation Methods in the wxEWA Program

Posters:

Miroslav Cukr, **P. Jiříček**, Igor Bartoš, J. Sadowski: Measurement of the Inelastic Mean Free Path for GaAs(100)-c(4x4) at Very Low Energies

J. Pavluch, Z. Pekárek, Y. Polyak, V. Stary: On the Low-Energy Electron Elastic Reflection from Some Materials – A Comparison of EPES Measurement and MC Simulation

K. Goto, Y.W.Li, Alakafri A. Ibrahimi, R. Shimizu: Aspect of Absolute AES; Work Function and Transmission

G. Gergely, G. T. Orosz, B. Lesiak, A. Jablonski, J. Tóth, D. Varga: Surface Excitation Correction of the Inelastic Mean Free Path of Selected Polymers

A. Jablonski, C. J. Powell: Monte Carlo Simulation of Electron Backscattering from Surfaces

J. Tóth, I. Cserny, L. Kövér, D. Varga: IMFP Measurements by XPS Using Different Energy X-rays

Z.M. Zhang, Z.J. Ding, R. Shimizu, T. Koshikawa, K. Goto: Effective Energy-Loss Functions Derived From REELS Spectra and Application to the Effective Depth of Surface Excitation

19.00 *Dinner*

20.30 – 21.30 Software Demonstration and Poster Session continues

Tuesday, July 6

9:00 – 10:35 V. Inelastic Scattering of Electrons in Solids 1.

Moderator: *S. Tanuma*

9:00 – 9:35 **S. Tougaard:** Intrinsic and Extrinsic Excitations in XPS and AES – *Invited Review*

9:35 – 9:50 F. Yubero, **S. Tougaard:** Quantification of Plasmon Excitations in Core-Level Photoemission

9:50 – 10:20 General Discussion

10:20 – 10:50 *Break*

10:50 – 12:25 VI. Inelastic Scattering of Electrons in Solids 2.

Moderator: *C.J. Powell*

10:50 – 11:25 **W.S.M. Werner:** Surface Effects in Electron Spectroscopy – *Invited Review*

11:25 – 11:40 **C. M. Kwei,** Y. H. Hsu, C. J. Tung: Memory Effect on the Inelastic Interaction of Electrons Moving Parallel to a Solid Surface

11:40 – 11:55 **T. Nagatomi:** Effects of Surface Excitations Deduced from Reflection Electron Energy Loss Spectra

11:55 – 12:25 General Discussion

12:25 – 14:00 *Lunch*

14:00 – 15:20 VII. Inelastic Scattering of Electrons in Solids 3.

Moderator: *C. M. Kwei*

14:00 – 14:35 **T. Fujikawa,** T. Konishi: Role of Interferences in Surface and Bulk Excitations – *Invited Review*

14:35 – 14:50 **J. L. Gervasoni:** Quantum Mechanical Calculations of Surface and Bulk Plasmon Excitations in Nano-Structures. Comparison with Classical Approaches

14:50 – 15:20 General Discussion

15:20 – 15.50 *Break*

15:50 – 17:40 VIII. Inelastic Scattering of Electrons in Solids 4.

Moderator: *M. Menyhárd*

15:50 – 16:25 **C. J. Powell:** Calculations of Electron Inelastic Mean Free Paths from Optical Data – Limitations and Comparison with Experiments – *Invited Review*

16:25 – 16:40 **S. Tanuma,** T. Shiratori, K. Goto, S. Ichimura, C. J. Powell, D. R. Penn: Calculations and Measurements of IMFPs in 13 Elements in the 50 –5000 eV Energy Range

16:40 – 16:55 **J. M. Sanz,** P. Prieto, E. Elizalde: IMFPs of α -Carbon, α -Boron and their Nitrides as Determined by Quantitative Analysis of REELS

16:55 – 17:10 **L. Glazov,** S. Tougaard: An Invariant-Embedding Technique for Detailed Analysis of Electron-Backscattering Distributions

17:10 – 17:40 General Discussion

19:00 *Dinner*

8:30 – 10:30 IX. Inelastic Scattering of Electrons in Solids 5. (EPES)

Moderator: *W. Werner*

8:30 – 8:45 **G. Gergely**, M. Menyhárd, S. Gurbán, J. Tóth, D. Varga, A. Jablonski: Surface Excitation Correction of the IMFP of Electrons Determined by EPES Experiments

8:45 – 9:00 **B. Lesiak**: Influence of Surface Excitation on the Electron IMFPs in Selected Elements and Polymers

9:00 – 9:15 **J. Zemek**: Photoelectron Escape from Iron Oxide

9:15 – 9:30 **A. Akkerman**: Inelastic Interaction of Charged Particles in Alkali Halides, Metal Oxides and Organic Compounds

9:30 – 9:45 **P. J. Cumpson**: Inelastic Electron Scattering: Quantitative Structure – Property Relationships and Monte Carlo Models

9:45 – 10:00 **M. Menyhárd**, A. Sulyok, K. Tókési: On the Applicability of the IMFPs Determined by Theoretical Calculations in Real Life Electron Spectroscopy

10:00 – 10:30 General Discussion

10:30 – 11:00 *Break*

11:00 – 12:00 X. Modeling of Electron Transport in Solids and Applications 1.

(Modeling of Electron Transport in AES and XPS)

Moderator: *T. Nagatomi*

11:00 – 11:15 **S. Tougaard**: Modeling of Electron Transport in Solids

11:15 – 11:30 **W.S.M. Werner**, W. Smekal, C. J. Powell: Modeling of Electron Transport in AES/XPS

11:30 – 11:45 **A. Akkerman**, J. Barak: Electron Interactions in Solids and Related Phenomena at Subexcitation Energies

11:45 – 12:00 **C. Cepek**: C₆₀ on Single-Crystal: Molecular Orientations Revealed by X-ray Photoelectron Diffraction

12:00 – 12:30 General Discussion

12:30 – 14:00 *Lunch*

14:00 – 15:10 XI. Modeling of Electron Transport in Solids and Applications 2.

Moderator: *S. Ichimura*

14:00 – 14:35 **M. Vos**: Modeling of Energy Loss and Elastic Scattering in Coincident Experiments – *Invited Review*

14:35 – 14:50 S. N. Samarin, O. M. Artamonov, A. D. Sergeant, **J. F. Williams**: Spin-Polarized (e,2e) Electron Scattering from W(110)

14:50 – 15:10 General Discussion

15:10 – 18:10 *City tour*

19:00 *Banquet*

9:00 – 10:35 XII. Modeling of Electron Transport in Solids and Applications 3.

Moderator: *M. Vos*

9:00 – 9:35 **M. El Gomati:** The Contrast Mechanism in Low and Very Low Voltage SEM –
Invited Review

9:35 – 9:50 **Z. J. Ding,** H. M. Li: Monte Carlo Simulation of SEM Images for Complex
Structures

9:50 – 10:05 **R. Gauvin:** Quantitative X-Ray Microanalysis of Real Materials Using Monte Carlo
Simulations

10:05 – 10:35 General Discussion

10:35 – 11:05 *Break*

11:05 – 12:30 XIII. Modeling of Electron Transport in Solids and Applications 4.

Moderator: *J. M. Sanz*

11:05 – 11:20 **P. M. Echenique,** A. Eiguren, V. M. Silkin, E. V. Chulkov, I. De Gurtubay,
J. M. Pitarke: Electron and Hole Dynamics at Bulk and Surfaces (presented by J. L.
Gervasoni)

11:20 – 11:35 **V. Starý,** J. Pavluch, J. Zemek: Monte-Carlo Simulation of Low-energy Electron
Elastic Reflection by Solids – Assessment by Experiment

11:35 – 11:50 **B. Gruzza,** P. Tomkiewicz, C. Robert-Goumet, L. Bideaux: Applied EPES and
M–M EPES Method in Surface Analysis

11:50 – 12:05 **K. Tókési,** X-M. Tong, C. Lemell, J. Burgdörfer: Surface Loss Functions at Large
Distances from Metal Surfaces

12:05 – 12:30 General Discussion

12:30 – 13:00 XIV. Closing Session

Moderator: *J. T. Grant*

Workshop Summary – *L. Kövér*

13:00 – 14:30 *Lunch*

List of participants

Dr. A. Akkerman	Yavne	Israel
Mr. Zoltán Berényi	Debrecen	Hungary
Dr. Cinzia Cepek	Trieste	Italy
Dr. István Cserny	Debrecen	Hungary
Dr. Peter J. Cumpson	Teedington	United Kingdom
Dr. Maurizio Dapor	Povo	Italy
Prof. Zejun Ding	Hefei	China
Mr. Sándor Egri	Debrecen	Hungary
Prof. Takashi Fujikawa	Chiba	Japan
Prof. Raynald Gauvin	Montreal	Canada
Dr. György Gergely	Budapest	Hungary
Dr. Juana Gervasoni	San Carlos de Bariloche	Argentina
Dr. Lev G. Glazov	Tomsk	Russia
Prof. Mohamed El Gomati	York	U. K.
Prof. K. Goto	Nagoya	Japan
Prof. John T. Grant	Dayton	U. S. A.
Prof. Bernard Gruzza	Clermont-Ferrand	France
Mr. Li Huimin	Hefei	China
Dr. Shingo Ichimura	Tsukuba	Japan
Prof. Alexander Jablonski	Warsaw	Poland
Dr. Petr Jiricek	Prague	Czech Republic
Dr. Masatoshi Jo	Tsukuba	Japan
Dr. Ranju Jung	Gyeonggi-do	Korea
Dr. László Kövér	Debrecen	Hungary
Prof. Cheng May Kwei	Hsinchu	Taiwan
Dr. Beata Lesiak	Warsaw	Poland
Prof. Hans-Jörg Mathieu	Lausanne	Switzerland
Dr. Miklós Menyhárd	Budapest	Hungary
Dr. Takaharu Nagatomi	Osaka	Japan
Dr. J. Pavluch	Prague	Czech Republic
Dr. Cedric J. Powell	Gaithersburg	U.S.A.
Prof. R. H. Ritchie	Oak Ridge	U.S.A.
Dr. Francesc Salvat	Barcelona	Spain
Prof. Jose M. Sanz	Madrid	Spain
Mr. Werner Smekal	Wien	Austria
Dr. Vladimir Stary	Prague	Czech Republic
Dr. Attila Sulyok	Budapest	Hungary
Dr. Shigeo Tanuma	Tsukuba	Japan
Dr. Károly Tókési	Debrecen	Hungary
Dr. József Tóth	Debrecen	Hungary
Prof. Sven Tougaard	Odense	Denmark
Prof. Chuan Jong Tung	Hsinchu	Taiwan
Dr. Dezső Varga	Debrecen	Hungary
Dr. János Végh	Debrecen	Hungary
Dr. Maarten Vos	Canberra	Australia
Dr. Dave Watson	Chanhassen	U.S.A.
Prof. Wolfgang Werner	Wien	Austria
Prof. Jim Williams	Perth	Australia
Dr. Josef Zemek	Prague	Czech Republic
Dr. Zengming Zhang	Hefei	China