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## Estimate of Control Voltage Tolerances for a Photo-Electron Analyzer of Toroidal Design

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We have run electron optics simulations and determined the tolerance in the control voltages of all elements (retarding input lens, analyzer, accelerating exit lens) of the La Trobe University photoelectron analyzer, recently redesigned to reach a spectral resolution of 5000, and which will be installed at LNLS (Campinas Brasil) and BESSY II (Berlin, Germany).

### 1 Introduction

Photoelectron spectroscopy is an important analytical technique based on the photo-electric effect. When an atom is illuminated with photons of sufficiently high frequency  $\omega$ , a bound electron of energy  $E_{\text{binding}}$  can be promoted to a free-state  $\mathbf{k}$  above the ionization threshold, with kinetic energy  $E_{\text{free}} = \hbar^2 k^2 / 2m_e = \hbar\omega - E_{\text{binding}}$ . Since, for a given  $\omega$ , there are in general many different core and valence levels with  $E_{\text{binding}} < \hbar\omega$ , one gets, from an energy analysis of the emitted photo-electrons, important information about the core and valence level positions and the density of states. There is ample literature covering the principles, instrumentation and “classical” analytical applications of photoelectron spectroscopy [1].

Further applications ensue in solid state physics and materials science. If, instead of a single atom, one considers a solid sample, then the exciting light might penetrate a few hundred atomic layers beneath the surface. The photoelectrons from deep layers, however, may interact strongly with the host crystal, suffer inelastic scattering and lose most of their kinetic energy before reaching the solid/vacuum interface. Only electrons emitted close to the surface make it to the vacuum outside and to the electron analyzer without undergoing inelastic scattering. The probability of escape is a sensitive function of the photoelectron initial kinetic energy. In this way, it is possible to contrive experimental conditions such that only photoelectrons from the surface layer itself escape, which lends to the photoemission experiment a unique surface-sensitive character.

The surface is of great fundamental interest because a real crystal grows from a seed by accretion of atoms at the surface; crystallization is a surface phenomenon.

In addition, it is of enormous technological interest, because the surface is the seat of all catalytic phenomena, on

which depend the chemical, pharmaceutical and petroleum industries.

Surface analysis is a very delicate business, because clean, well characterized surfaces are difficult to prepare and to keep for extended periods of time. Even in the highest quality vacuum possible with current technology (say,  $10^{-11}$  mbar pressure with mainly H as residual gas) a clean surface becomes contaminated with adventitious residual atoms and molecules in a few hours. It is, therefore, mandatory to complete the photoelectron data gathering in a shorter time.

The photoelectron detection rate depends on many parameters, including energy and angle resolution of the electron energy analyzer, cross-section for photoemission of the particular chemical species under study, frequency intensity and polarization of the photon-source, etc, but it is usually much lower than desirable.

There is a constant striving to get more and more intense photon sources - the state of the art today is to use undulator radiation from a low emittance synchrotron source [2,3].

On the opposite end of the chain, parallel detection of photoelectrons in an extended angular and energy range is obviously a desirable and efficient way of gathering data.

Many different schemes of parallel detection have been proposed and demonstrated [4]. Here, we are interested in the toroidal analyzer designed at La Trobe University, Melbourne, Australia. This device was described several years ago [5], and a new version with much improved spectral and angular resolution has been designed recently and is scheduled for tests at the 3<sup>rd</sup> generation synchrotron light facility BESSY II (Berlin, Germany) in the first semester of 2003, and also for installation at LNLS and elsewhere in the near future. The optimum control electronics for this detector is still under discussion in what concerns cost/performance ratio, and this is the subject of this paper.

Figure 1 shows a photograph, and Fig. 2 a cross-section of the analyzer, which has cylindrical symmetry about the vertical axis. Electrodes 1 2 3 belong to an entrance retarding lens. They focus a beam of photo-emitted electrons covering a zenithal angle interval  $\Delta\Theta$ , coming from a sample placed on axis. This focusing is done independently and simultaneously for all azimuthal angles  $0 < \Phi < \pi$  of emission from the sample. The analyzer proper is a pair of concentric toroids kept at different electric potentials. An almost radial electric field exists in the region between the toroids, which deflects the electrons. The total deflection at the exit of the toroidal section is roughly proportional to the time-of-flight, i.e. to  $E_{\text{kinetic}}^{-1/2}$ . An approximate analytical model of the fields in the toroidal section has been given by the La Trobe team [6]. An accelerating exit lens boosts the kinetic energy of the analyzer output (for more efficient generation of secondary electrons) and refocus it on a Microchannel electron multiplier plate. The intensified electron cloud then falls on a fluorescent screen. The visible light emitted by each pixel is read out by a CCD camera and gives the number of detected photoelectrons in a range  $\Delta E$  of energy and  $\Delta\Theta \Delta\Phi$  of zenithal and azimuthal angles. This image, with about  $4 \cdot 10^6$  pixels  $20 \times 20 \mu\text{m}^2$  each, is stored on disk for further off-line analysis.



Figure 1. Photograph of the La Trobe photoelectron toroidal analyser.

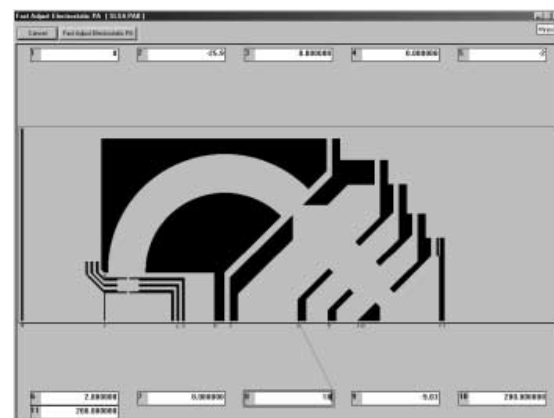


Figure 2. Cross-section of the La Trobe photoelectron toroidal analyser.

## 2 Methods

The effects of fluctuations (noise) on the electrical voltages of the eleven control electrodes are vastly different, depending on function and position of the electrode.

The cost of a power supply increases steeply as one tries to reduce the noise. It is, therefore, of critical interest to determine the largest tolerance the power supplies might admit for a (small) given loss in the optimum ideal performance. We took as ideal starting point the spectral resolving power of 5000, limited by aberrations in the electron optics, and the voltages prescribed by Tadich, Riley and Leckey [7], making an allowance of 20 % increase or displacement in the focal spot. We then found the permissible tolerance for the voltage of each electrode under a variety of conditions.

The electron spot size and position in the detector plane were studied with the commercial program SimIon [8]. This program, initially developed at La Trobe University, then sold to a private US company, calculates the potential  $V(\mathbf{r})$  in the vacuum region between the electrodes using the potentials given at the electrodes as boundary conditions. The solution to the Laplace equation is found using a relaxation technique, with various enhancements to speed up the convergence of the method. Once the electric field  $-\nabla V(\mathbf{r})$  is obtained, the equation of motion for each photoelectron with given initial conditions is numerically solved and the trajectory tracked till the electron strikes the MCP detector. In order to reach acceptable accuracy, very small time increments have to be specified in the numerical solution of the equation of motion, which leads to many weeks spent on these simulations.

## 3 Results

It is possible to determine the effect of the variation of the voltage on an electrode by holding all the other electrode

voltages constant and observing the changes in resolution for changes in that electrode's voltage.

Figure 3 shows the effect of voltage changes in  $V_1$ . This is the first element of the retarding entrance lens and has the function of retarding the incoming electron to the kinetic energy of the central orbit in the toroidal analyzer, which is the *pass energy* of the analyzer. If the pass energy is kept fixed and the electron kinetic energy is varied, we expect the radius of curvature of the trajectory to change (increasing for larger energies, being reduced for lower energies) and the edges of the focal spot to move radially on the MCP detector, in a fashion approximately linear with changes in the kinetic energy. This is clearly seen in the figure, from which one can also extract a linear deviation coefficient  $dr/dV_1 \approx -42 \text{ mm/V}$ . Then one finds the voltage tolerance  $\Delta V_1$  by requiring that  $\Delta r$  be at most 20% of the optimum spot size.

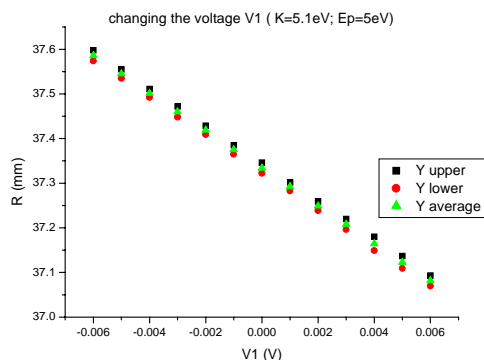


Figure 3. Dependence of the position of the focal spot on the voltage applied to electrode  $V_1$ . "Upper" and "Lower" refer to the radial edges of the electron focal spot, while "Average" refers to the estimated radial position of the centroid.

Figure 4 shows the effect of voltage changes in  $V_2$ . This is the "focusing" element of the retarding entrance lens. As the voltage departs from the optimum value, the spot increases in size, without significant radial motion of its centroid, as expected. Here, again, the voltage tolerance is chosen to be that  $\Delta V_2$  which increases the spot size by 20%.

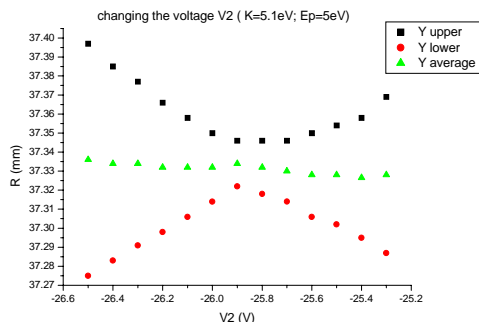


Figure 4. Dependence of the focal spot size on the voltage applied to electrode  $V_2$ . "Upper" and "Lower" refer to the radial edges of the electron focal spot, while "Average" refers to the estimated radial position of the centroid.

Figure 5 shows the tolerance on voltage  $V_1$  as a function of incoming photoelectron energy, for various pass energies.

It is interesting to observe that the tolerance is substantially smaller than the naïve estimate of  $\Delta V_1/V_1 \approx \Delta E/E \approx 1/5000$ .

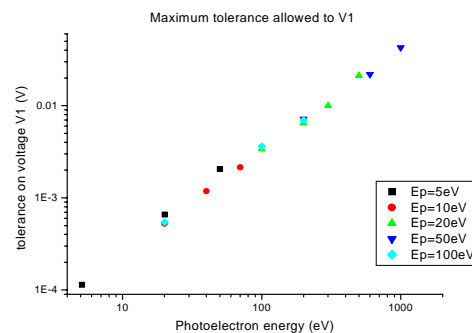


Figure 5. Tolerance on the voltage applied to electrode  $V_1$  in order to have a loss in spectral resolution not exceeding 20%, as a function of incoming electron kinetic energy, for various pass energies. This is a retarding electrode.

The value of the focusing element  $V_2$  voltage is not critical, requiring a power supply with a precision of only a few percent.

$V_5$  and  $V_6$  are the analyzer toroids. For low kinetic energy, the required precision is high, being about  $8 \cdot 10^{-5}$   $V_6$ , again much tighter than the naïve  $1/5000$ . This is shown on Figure 7.

The focusing electrode  $V_8$  in the exit lens is also very undemanding, a precision of a few percent is satisfactory, as shown in Figure 6 (open symbols).

The electrode  $V_9$  needs a precision of roughly 1 part in 1000 in the worst case, see Figure 6 (full symbols).

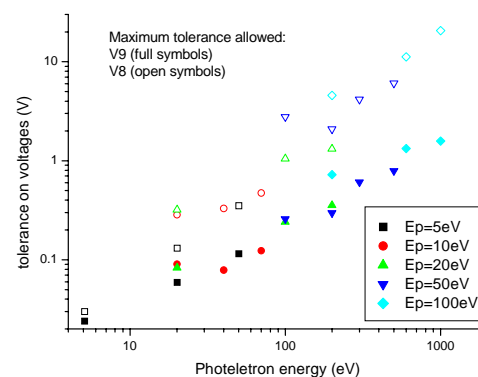


Figure 6. Open symbols: tolerance on the voltage applied to electrode  $V_8$  in order to have a loss in spectral resolution not exceeding 20%, as a function of incoming electron kinetic energy, for various pass energies. Full symbols: tolerance on the voltage applied to electrode  $V_9$ . These are focussing electrodes in the exit lens.

Finally, voltage fluctuations on the equipotential electrodes  $V_{10}$  and  $V_{11}$  (the last one is the MCD detector surface) have very small effects.

In this analysis we ignored the azimuthal focusing because this has no effect on radial focusing and only a small effect on the azimuthal angular resolution that is usually not critical. In fact, binning of azimuthal pixels is routinely used

to speed up the data transfer between CCD camera and the control computer, and to reduce the volume of data stored and treated.

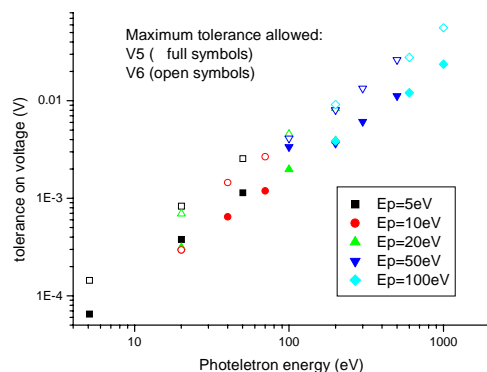


Figure 7. Tolerance on the voltage applied to electrode V<sub>5</sub> (full symbols) and electrode V<sub>6</sub> (open symbols) in order to have a loss in spectral resolution not exceeding 20%, as a function of incoming electron kinetic energy, for various pass energies. These are the toroidal energy-dispersive electrodes.

## 4 Conclusions

We have run computer simulations of the electron trajectories in a complex photoelectron analyzer of toroidal geometry with input and output lenses, in order to establish tolerances for the control voltages of the electrodes. We find

that, contrary to naïve expectation, the precision required on the energy selecting electrodes is much finer than  $\Delta E/E \approx 1/5000$ , the maximum spectral resolution allowed by aberrations of the electron optics, which is roughly consistent with the spatial resolution dictated by MCD size, and the CCD camera number ( $4 \cdot 10^6$ ) and size of pixels.

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