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Modelling the line shape of very low energy peaks of positron beam induced secondary electrons measured using a time of flight spectrometer

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Abstract. In this paper, we present results of numerical modelling of the University of Texas at Arlington's time of flight positron annihilation induced Auger electron spectrometer (UTA TOF-PAES) using SIMION® 8.1 Ion and Electron Optics Simulator. The time of flight (TOF) spectrometer measures the energy of electrons emitted from the surface of a sample as a result of the interaction of low energy positrons with the sample surface. We have used SIMION® 8.1 to calculate the times of flight spectra of electrons leaving the sample surface with energies and angles dispersed according to distribution functions chosen to model the positron induced electron emission process and have thus obtained an estimate of the true electron energy distribution. The simulated TOF distribution was convolved with a Gaussian timing resolution function and compared to the experimental distribution. The broadening observed in the simulated TOF spectra was found to be consistent with that observed in the experimental secondary electron spectra of Cu generated as a result of positrons incident with energy 1.5 eV to 901 eV, when a timing resolution of 2.3 ns was assumed.

1. Introduction

The UTA TOF-PAES is capable of generating and transporting a very low, ~1 eV, positron beam and detecting the subsequent electrons emitted from the sample with energy as low as ~0 eV. The spectrometer consists of: (1) a permanent neodymium magnet behind the sample used to parallelize the ejected electron momentum, (2) a field free TOF tube, (3) a set of $\mathbf{E} \times \mathbf{B}$ plates that deflects electrons onto a micro-channel plate (MCP), and (4) detector electronics used in determining the TOF. The energy of the incident positron beam can be adjusted by applying a voltage bias to the sample, resulting in incident positron beam energies of ~1.5 eV to ~901 eV [1].

The work in this paper was motivated by the desire to better understand the nature of the spectrometer's instrument response function in order to obtain a quantitative estimate of the true energy spectrum of low energy electrons emitted from a polycrystalline Cu sample as a result of Auger mediated positron sticking (AMPS) and related positron induced electron emission processes [2].

2. TOF-PAES Spectrometer Model

The measured TOF distribution of electrons emitted from the sample surface is broadened by the instrument response function of the TOF-PAES spectrometer. The parameters that determine this broadening include: (1) the magnetic field gradient produced by the permanent magnet behind the sample, (2) the electric fields along the flight path of the electrons, and (3) the timing resolution of the detection electronics [3]. SIMION® 8.1 simulations, using the experimental parameters listed in table 1, were used to model the TOF broadening due to the combined effect of the magnetic gradient and the perpendicular electric and magnetic fields between the **E**×**B** plates. A more detailed description of the experimental system modelled can be found in reference [1].

Single energy electrons generated randomly on a 2.6 mm diameter circle and emitted with isotropic angular distribution, were flown in the SIMION® 8.1. The TOF of the electrons reaching the MCP was calculated using reverse timing to be consistent with the timing scheme adopted in the experiment and was counted to generate a histogram. That way low time of flights correspond to lower energies and high time of flights correspond to higher energies as is the case in the experiment. The modelled TOF spectrum was then convolved with a Gaussian function, meant to represent the timing resolution of the TOF system, and was converted to the energy domain using an experimentally derived conversion formula. The output of the simulated spectrometer, to the input delta function energy distributions, was used to obtain the broadening of trial functions, representing the true secondary electron distribution, using the principle of superposition. The timing resolution function used was a ~2.35 ns (FWHM) Gaussian which was found by convolving the simulated secondary electron TOF data, for electrons generated as a result of positrons incident with ~901 eV, with a series of Gaussians of different FWHMs until a match with experiment was found.

Table 1. Experimental parameters used in the SIMION® 8.1 model of the TOF-PAES spectrometer. The axial magnetic field is the magnetic field along the beam axis (south to north), the sample magnetic field is the magnetic field measured at the sample surface, and the east and west **E**×**B** plates refer to the plates east and west of the beam axis. See reference [1] for further details regarding the experimental apparatus.

Experimental Parameters	Value
Axial Magnetic Field	0.004 T
Sample Magnetic Field	0.046 T
East **E**×**B** Plate Voltage	-2.79 Volts
West **E**×**B** Plate Voltage	+3.19 Volts
E×**B** Plate Length	0.267 m
E×**B** Plate Spacing	0.025 m
Sample to MCP Distance	1 m

3. Results and Discussion

The choice of trial energy distribution functions used as inputs in our simulations was guided by the relevant physics of the positron induced electron processes measured. Following previous studies, we started with a parameterized trial function which has been used to describe the spectra of true secondary electrons produced by an electron beam [2, 4].

$$\mathrm{N}(E) = A \frac{E}{(E + E_0)} (E + \varphi)^m \qquad (1)$$

The terms E_0, φ, and m are fitting parameters and were optimized to match the experimental data. Two regimes of parameters were found to match experiment best: (1) E_0 = .35 eV, φ = 4.6 eV, m = -2.5 and (2) E_0 = .35 eV, φ = 4.6 eV, m = -1.6.

If a positron transitions from a positive energy scattering state to the bulk ground state, then the maximum kinetic energy of the emitted secondary electron is given as:

$$\mathrm{E_{kin}} = E_{e+} + \varphi^{+}_{samp} - \varphi^{-}_{samp} \qquad (2)$$

where E_{e+} is the maximum kinetic energy of the positron incident on the sample taking into account the maximum kinetic energy of the positron inside the TOF tube, the contact potential between the sample and sample chamber, and the sample bias, φ^{+}_{samp} is the positron work function, and φ^{-}_{samp} is the electron work function. However, if the incident positron becomes trapped in a surface state directly from the scattering state then the maximum kinetic energy of the emitted electron is given as:

$$\mathrm{E_{AMPS}} = E_{e+} + E_{b} - \varphi^{-}_{samp} \qquad (3)$$

where E_{b} is the surface state binding energy. This AMPS mechanism is dominant at very low energies but does not make a significant contribution to the electron yield for incident positron energies above ~10 eV [2, 5]. The function in equation 1 cuts off at an energy determined by equation 2 or 3 depending on the maximum incident positron energy. Using equation 2, which represents the most probable process of electron emission at incident positron energies > 10 eV, we find the maximum kinetic energy for secondary electrons due to 901.25 eV positrons incident on a polycrystalline Cu to be 896.6 eV (taking φ_{cu}^{-} = 4.65 eV and φ_{cu}^{+} = 0 eV) [6]. Using the equation relevant at low positron energies, equation 3, we find the maximum kinetic energy for secondary electrons due to 3.75 eV positrons incident on a polycrystalline Cu sample to be 1.74 eV (taking E_{b} = 2.64 eV) [1].
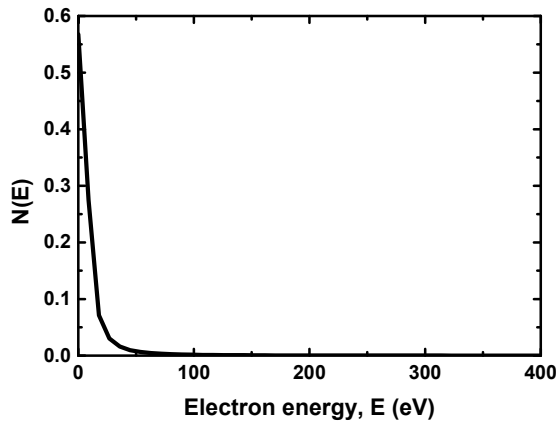

Figure 1. Electron energy distribution which was input to the simulated TOF spectrometer. This was chosen to represent the true energy distribution of secondary electrons from Cu for positrons incident at 901.25 eV. The distribution was generated using equation 1 with E_{0} = .35 eV, φ = 4.6 eV, m = -2.5. The maximum secondary electron energy was calculated as 896.6 eV using equation 2.
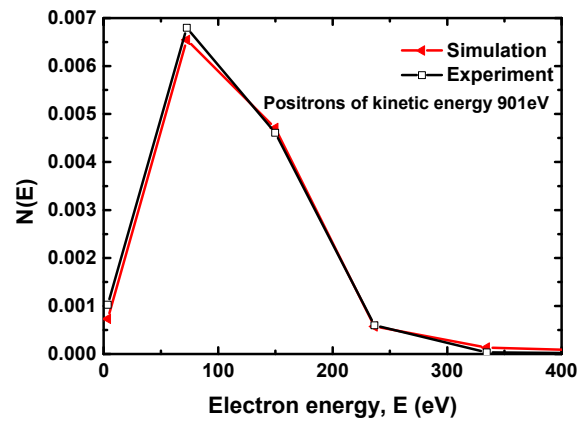
Figure 2. Comparison of the experimental and the simulated energy spectra of positron induced secondary electrons from the surface of a polycrystalline Cu at an incident positron energy of 901.25 eV. The legend indicating positron energy does not include the effect of contact potential. The simulated TOF spectrum was convoluted with a Gaussian of FWHM ~ 2.35 ns before conversion into energy.
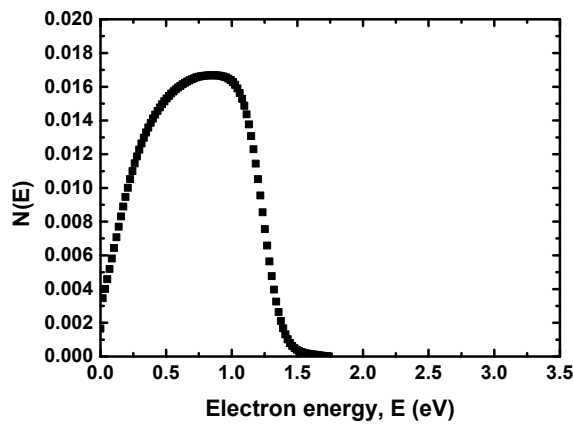
Figure 3. Electron energy distribution which was input to the simulated TOF spectrometer. This was chosen to represent the energy distribution of electrons emitted from Cu as a result of the sticking of 3.75 eV positrons on surface via AMPS process. The distribution was generated using equation 1 with E_0 = .35 eV, φ = 4.6 eV, m = -1.6. The maximum electron energy was calculated as 1.74 eV using equation 3.
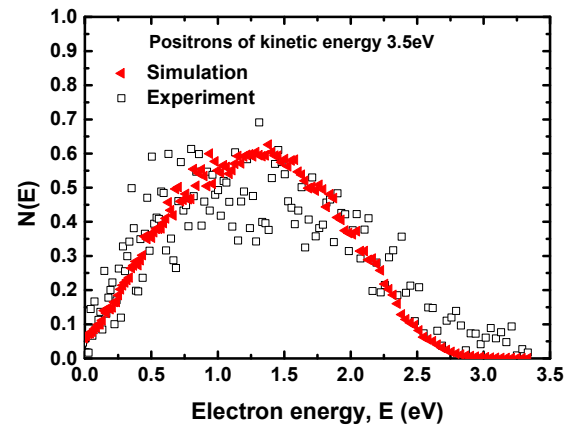
Figure 4. Comparison of experimental and simulated energy spectra of positron induced electrons from the surface of a polycrystalline Cu sample through the AMPS process. The legend indicating positron energy does not include the effect of contact potential. The simulated TOF spectrum was convoluted with a Gaussian of FWHM ~ 2.35 ns before conversion into energy.

Figure 1 shows the input electron energy distribution function, based on equation 1 with E_0 = .35 eV, φ = 4.6 eV, m = -2.5, for secondary electrons generated as a result of positrons incident with energy 901.25 eV. Figure 2 compares the respective simulated output with experimental Cu data. Figure 3 shows the input electron distribution function, based on equation 1 with E_0 = .35 eV, φ = 4.6 eV, m = -1.6 for electrons generated as a result of positrons incident with energy 3.75 eV. Figure 4 shows the simulated output compared with experimental Cu data. 50,500 particles were flown with the input electron energy distributions (figures 1 and 3) taking into account the distribution in the energy of positrons incident on the sample through a convolution of equation 1 with a Gaussian centred at ~0.5 eV and having a FWHM of 0.26 eV. The measured energy spectra can be seen to be significantly broadened in energy as compared to the model input spectra shown in figures 1 and 3. This broadening is well accounted for by the instrumental broadening found from our numerical modelling over a wide range of electron energies (~0.5 eV to ~900 eV) when a timing resolution of 2.35 ns was assumed.

4. Conclusion

In this paper, we have presented a model simulation of the University of Texas at Arlington's time of flight positron annihilation induced Auger electron spectrometer using SIMION® 8.1. Using this model we have determined the timing resolution of our system to be 2.3 ns. A parameterized function, equation 1, was used to model the initial kinetic energy of secondary electrons leaving the Cu sample as a result of positron annihilation inside the material. After comparison with experimental data, two regimes of parameters were found to match experiment best, one for incident positron energies above ~10 eV and one for incident positron energies below ~10 eV. We believe regime 1 to represent positrons which mostly transition from a scattering state to a bulk state before thermalization and annihilation in a surface state while regime 2 represents positrons which mostly transition from a scattering state directly to a surface state. However, more work needs to be done in order to verify this.

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