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LETTER TO THE EDITOR

Positron backscattering probabilities from solid surfaces at 2–30 keV

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Abstract. A measurement of the total positron backscattering probabilities using a magnetically guided positron beam is reported. Backscattering yields were measured as a function of the incident positron energy in the range 2–30 keV and the atomic number Z of the target ($6 \leqslant Z \leqslant 79$). Absolute backscattering probabilities extracted from the annihilation count rates at the target are compared with doubly differential measurements at 35 keV. The total backscattering ratios from these two measurements agree within the experimental uncertainties. The experimental backscattering probabilities compare well with Monte Carlo simulations of keV positron slowing in solids.

As keV positron beams are applied as analytical probes to study solid surfaces, thin films and interfaces (Schultz and Lynn 1988, Schultz *et al* 1990), there is a practical motivation to determine the absolute positron backscattering probabilities. There are differences in the interactions of energetic electron and positron beams with solid surfaces. The backscattering probability for keV positrons is only about half of that for electrons, as determined by Monte Carlo simulations (Valkealahti and Nieminen 1983, 1984, Valkealahti 1987). The backscattering probability is the most accurate quantity for a direct comparison of Monte Carlo simulations of keV electron and positron slowing in solids with experiments. Experimental backscattering ratios therefore serve also as a test of the theoretical models of the interaction of keV electrons or positrons with solids.

So far only a few published results exist for positron backscattering at solid surfaces at keV energies. Mills and Wilson (1982) reported a measurement of backscattering yields in Al films at incident positron energies below 3 keV. The only systematic measurements of positron backscattering are those of Baker and Coleman (1988) and Massoumi *et al* (1991). Baker and Coleman (1988) reported the first measurements of the total backscattering ratios in the energy range 0.5–30 keV. Massoumi *et al* (1991) measured the energy and angular distributions of backscattering for 35 keV incident positrons using an electrostatically guided positron beam. The results of these two measurements deviate significantly from experiments performed using high energy ($E > 100$ keV) positrons. Some of those differences were shown to arise from the diffuse angle of incidence in the experiments at beta-decay energies (Massoumi *et al* 1991). However, the backscattering ratios reported by Baker and Coleman and Massoumi *et al* differ also from each other. The latter experiment yields systematically higher values, thereby indicating the present uncertainty in the absolute backscattering probabilities in particular at the incident energies $E < 10$ keV.

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In the present work, we have studied positron backscattering for normal incidence at solid surfaces as a function of the incident energy in the range 2–30 keV and the target atomic number $6 \leqslant Z \leqslant 79$. It appears that with our present set-up of the magnetically guided positron beam the total numbers of annihilation events at the target are in agreement with much more elaborate measurements of the backscattering probabilities (Massoumi *et al* 1991) and can be used to extract the total backscattering ratios. The magnetically transported beam does not allow for the measurement of differential backscattering distributions as the energy and scattering angle cannot be distinguished unambiguously in the magnetic field. However, the *total* backscattering ratio can be measured directly and we can also extend the experiment to low incident positron energies. In principle the experiment is very similar to that of Baker and Coleman (1988).

We have also carried out Monte Carlo simulations of positron slowing in solids. The simulations were done using the computer code of Valkealahti and Nieminen (1983, 1984). Generally speaking, the absolute backscattering probabilities and their energy dependence are in good agreement with the experiment.

The magnetically guided positron beam used in the experiment is described in detail elsewhere (Lahtinen *et al* 1986). Positrons from an encapsulated ^{22}Na source are moderated in a 0.7 μm W(100) single-crystal foil which has a negative positron affinity. The energy of re-emitted positrons is equal to the work function, $|\phi_+| \approx$ 3 eV. After passing through the velocity filter, the beam is accelerated to the final energy from 100 eV to 30 keV in an electrostatic accelerator. The magnetic field strength at the target position was raised to 400 G compared to 70 G in the transport line using a permanent magnet behind the target. The intensity of the beam at the target was approximately 8×10^5 e^+ per s, and the beam diameter was less than 4 mm. The base pressure of the chamber was 5×10^{-8} mbar.

The backscattering yields were measured for polyethylene (PE), highly oriented pyrolitic graphite C, Si(100), Co(11$\bar{2}$0), Ni(100), Cu(111), Ge(surface orientation not known), Mo(110), Cd(0001), W(100) and polycrystalline Au. The sample holder could carry five samples at a time. The sample surfaces were not cleaned *in situ*. Because of the Larmor motion, the angle of incidence is not strictly normal to the surface of the target, but from any reasonable estimates of the transverse energy of the beam the angle of incidence deviates from the normal direction by less than 5° when the incident energy is $E \geqslant 2$ keV. The annihilation radiation was detected with a high-purity Ge detector 50 mm from the target. When all the incident positrons were made to annihilate at the target, the count rate was 1.58×10^4 s^{-1}. The total number of counts in the spectra varied from 4.8×10^5 to 8.0×10^5 depending on the backscattering yield, i.e. the target material and the incident positron energy.

The backscattering ratios η at each incident energy were extracted from the number of annihilation events simply as $N = N_0(1-\eta)$, where N_0 is the total number of annihilations when all incident positrons annihilate at the target. A precise measurement of the intensity of the incident beam is a precondition for the measurement of the absolute backscattering ratios. To find N_0, we used a grid biased to 50–500 V below the incident beam energy in front of a low-Z target, PE (in PE the backscattering ratio is $\eta = 0.06\pm0.02$) to turn the backscattered positrons to the target. From 1 to 10 keV the total count rate was independent of the incident energy. At higher energies $E > 10$ keV, N_0 could not be directly measured. For low-Z materials like PE and graphite in which the backscattering is expected to be a very weak function of the incident energy, the total number of counts varied less than $\pm1\%$ from 2 to

30 keV. We conclude that any systematic variations of the incident beam intensity are no more than ±1% over the energy range 2–30 keV.

Another source of systematic error comes from the possible detection of the annihilation radiation from the backscattered positrons. The magnetic field strength of approximately 400 G at the target position is sufficient to guide all the backscattered positrons back to the beam line when their maximum energy is 30 keV or less (the Larmor radius $r_L < 15$ mm). In the beamline the field strength decreases to 70 G increasing the radius of Larmor motion. Therefore, the majority of the backscattered positrons annihilate on an aperture plate at a distance from the detector for which the number of annihilation events detected is negligible. Only those positrons scattered close to the normal direction can pass the aperture, and their final annihilation site is not known. One can roughly estimate their contribution assuming a cosine angular distribution of backscattered positrons and the shape of the energy distribution from experiments or Monte Carlo simulations (Massoumi *et al* 1991, Valkealahti and Nieminen 1983, 1984). At 5 keV the fraction is 10% or less of the total backscattering ratio, and at 30 keV it is less than 2%. The systematic errors due to possible detection of the annihilation radiation from the backscattered positrons are at most approximately equal to the uncertainties in the count rates.

The experimental backscattering probabilities reported below include positrons which leave the sample with energies higher than 20 eV. The emission of epithermal positrons at eV energies was prevented by applying +20 V to the grid in front of the sample. The grid was at a distance from the detector for which the detection efficiency is negligible. We have only included data from incident energies above 2 keV. At lower energies there are complications arising from positronium (Ps) formation at the surface, and the sensitivity of low-energy positrons to the surface condition. At clean metal surfaces Howell *et al* (1986) have reported Ps formation by backscattered positrons by measuring the Ps time-of-flight in vacuum. Its total intensity for 2 keV incident energy is 5% or lower. In the present experiment we could not detect any Ps formation at the incident energies $E > 2$ keV, as judged from the annihilation energy spectrum.

We estimate that the overall uncertainty in the absolute backscattering probability is $\Delta\eta = \pm\, 0.02$. For high-Z targets the experimental uncertainty is less than 10% of the backscattering probability. For $Z < 20$, the uncertainties are larger, increasing up to 30% in the cases of PE and graphite because of their small backscattering ratios. The overall experimental uncertainties are essentially equal to those in other experiments (Baker and Coleman 1988, Massoumi *et al* 1991).

Figure 1 shows the total backscattering probabilities at the incident positron energies 4.8 and 30 keV. The target atomic number varies from Z = 6 (graphite) to Z = 79 (Au). In the same figure the backscattering ratios reported by Massoumi *et al* (1991) are given. The incident energy in the latter measurement was 35 keV but the variation of η with energy is very small in this energy range (Kuzminikh *et al* 1974) justifying the direct comparison of the backscattering probabilities.

At 30 keV the backscattering probability increases from $\eta = 0.06\pm0.02$ in graphite to 0.39 ± 0.02 in Au. The result is in very good agreement with the total backscattering probabilities integrated from the differential energy and angular distributions (Massoumi *et al* 1991). In the whole range of target atomic numbers from Z = 6–79 the absolute backscattering ratios as given by these two experiments are equal within the experimental uncertainties. However, our data indicates systematically higher backscattering probabilities than those reported by Baker and Coleman (1988).

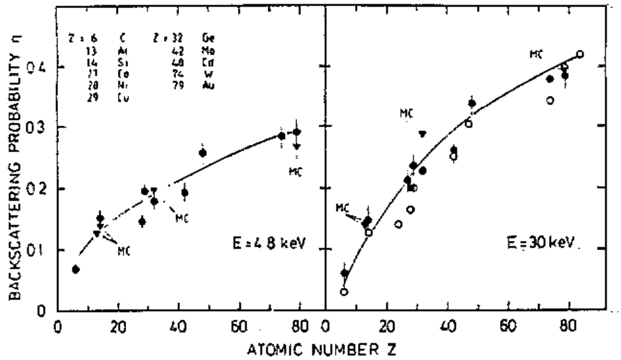

Figure 1. Total positron backscattering probabilities η for semi-infinite targets as a function of the target atomic number for 4.8 and 30 keV incident energies (●). Results from Monte Carlo calculations at 5 and 30 keV (▼) and the backscattering ratios integrated from differential measurements at 35 keV (○) (Massoumi *et al* 1991) are also shown.

For electron backscattering from semi-infinite targets, Arnal *et al* (1969) introduced an empirical relation $\eta = 1/(1 + \cos\theta_i)^p$ with $p = \alpha/Z^{1/2}$ to describe the backscattering probability of semi-infinite targets as a function of the target atomic number and angle of incidence θ_i. For normal incidence it takes the form $\eta = 2^{-p}$. For electrons at incident energies $E > 10$ keV, $p = 9.4/Z^{1/2}$ accounts for the experimental backscattering ratios to a good approximation for a large range of target atomic numbers and the angle of incidence $0° \leqslant \theta_i < 90°$ (Niedrig 1982). The solid line in figure 1 is calculated using the same relation but with $p = 11.5/Z^{1/2}$ for 30 keV positrons. For 4.8 keV incident positrons, the dependence of the total backscattering on the target atomic number is significantly weaker. This is because of the smaller backscattering probability from high-Z targets.

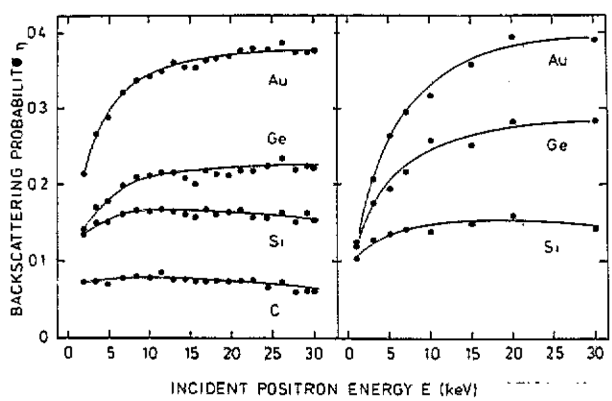

Figure 2. Left: experimental positron backscattering probabilities as a function of the incident energy for graphite, Si, Ge and Au. The estimated overall uncertainty of the absolute backscattering ratio is ±0.02. Right: positron backscattering probability from Monte Carlo calculations for Si, Ge and Au at incident energies 1–30 keV.

Figure 2 shows the energy dependence of the total backscattering ratios at the incident energies 2–30 keV for graphite, Si ($Z = 14$), Ge ($Z = 32$), and Au. Similar data from Monte Carlo simulations over the energy range 1–30 keV are shown for Si, Ge and Au (see below). In low-Z materials like PE, graphite or Si the variation of η with the incident energy is very small. At incident energies $E > 10$ keV, η saturates and gradually starts to decline. The energy dependence becomes stronger at target atomic numbers $Z > 20$ indicating an increase of the backscattering ratio as a function of the incident energy. In the high-Z targets like W or Au the backscattering probability saturates above 20 keV.

We also show the results of Monte Carlo (MC) simulations of positron backscattering for Al, Si, Ge and Au in figures 1 and 2. The simulations were done using the computer code of Valkealahti and Nieminen. The scattering cross sections and the simulation procedure are described in detail in the literature (Valkealahti and Nieminen 1983, 1984). In particular, the elastic scattering processes are calculated using accurate atomic cross sections modified to include the effect of the lattice structure approximately. The simulation was terminated when the positron energy was 20 eV. Typically 2×10^3 and in some cases 10^4 particle histories were followed. The incident energy in the simulation was extended from 10 keV (Valkealahti and Nieminen 1983, 1984) to 30 keV.

Generally, there is fair agreement between the experimental and simulated total backscattering ratios. At low incident energies and low-Z targets the simulation reproduces the experimental results with very good precision. At 5 keV, the backscattering probabilities as given by the MC calculation are equal to the experimental values within the experimental uncertainties from $Z = 13$ to $Z = 79$ (figure 1). For Si the simulated and experimental backscattering probabilities are equal to the whole energy range 2–30 keV (figure 2). Some discrepancies appear at heavier elements at higher incident positron energies. The differences are most pronounced at the target atomic numbers around $Z = 30$. This is seen in the case of Ge ($Z = 32$). For 30 keV incident positron energy the backscattering probability from the MC calculation is higher than the experimental one by a factor of ~ 1.3. The same conclusion can be made if one compares the experimental results with the MC simulation of positron backscattering due to Jensen *et al* (1990). The difference appears to be significant as the same is seen in the results of Massoumi *et al* (1991). The agreement between MC calculations and the experimental backscattering probabilities gets clearly better again at high-Z targets as one can see by comparing the results for Au in figures 1 and 2. The experimental backscattering probabilities in figure 2 show a much stronger dependence on the incident energy than those reported by Baker and Coleman (1988) but compare well with the results of MC calculations.

The backscattering probabilities from semi-infinite targets are significantly higher for electrons than for positrons. Massoumi *et al* (1991) found the ratio of electron and positron backscattering probabilities η^-/η^+ to be approximately 1.3 for 35 keV incident particles in agreement with the values found at beta-decay energies (Kuzminikh *et al* 1974). These observations suggest that the ratio η^-/η^+ depends very little on the target atomic number or the incident energy above a few tens of keV (Massoumi *et al* 1991).

At incident energies $E < 10$ keV, the electron backscattering ratios decrease much less than those for positrons, and for low-Z targets the electron backscattering actually increases (Fitting 1974, Massoumi *et al* 1990, Valkealahti and Nieminen 1983, 1984). At 2 keV the reported electron backscattering coefficients for Al and Au are $\eta^- = 0.21$ (Fitting 1974) and $\eta^- = 0.45$ (Schou and Sorensen 1978), respectively. Taking the experimental data for positrons from figure 2 (assuming that the backscattering ratio for Al is equal to Si which is justified by the simulations), the ratios η^-/η^+ are 1.6±0.3 for Al and 2.0±0.2 for Au. The results are in agreement with MC calculations (Valkealahti and Nieminen 1983, 1984) from which one can estimate the corresponding values 1.75 (Al) and 2.1 (Au). The difference between positron and electron backscattering can be understood in terms of their elastic scattering cross sections at keV energies, in particular the larger total elastic scattering cross section of electrons and their larger relative probability to undergo large angle scattering events. This matter has been discussed in detail elsewhere (Valkealahti and Nieminen 1983, 1984). Part of the difference is also due to the energetic secondary electrons, but their contribution to the experimental electron backscattering probability is typically less than 10% (Kalef-Ezra *et al* 1982).

In summary, total positron backscattering probabilities were measured for semi-infinite solid targets in the energy range 2–30 keV. Using a magnetically guided positron beam, the total backscattering ratios were extracted from the numbers of annihilation events at the target. The results are in good agreement with the total backscattering probabilities at 35 keV integrated from the differential energy and angular distributions (Massoumi *et al* 1991). We also compared the results with Monte Carlo simulations of positron slowing in solids (Valkealahti and Nieminen 1983, 1984). The experimental backscattering coefficients are compatible with the present understanding of elastic and inelastic scattering processes and the stochastical description of positron transport implied by the Monte Carlo method. At least there is no gross disagreement between the two at keV energies.

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