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Low-Energy Positron Diffraction from a Cu(111) Surface

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The first observation of low-energy positron diffraction from a solid surface is reported. Slow (20–400-eV) monochromatic positron beams were focused onto a Cu(111) surface and their elastically scattered distributions detected with a channel electron multiplier. Measurements of the scattered intensity versus angle as a function of incident energy show peaks at the predicted $(0\bar{1})$ and $(0\bar{2})$ diffraction angles. Profiles of intensity versus energy at fixed angles exhibit maxima corresponding to the primary Bragg peaks.

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In this Letter we report the first observation of low-energy positron (e^+) diffraction (LEPD) from a solid surface, Cu(111).[1] LEPD offers the possibility of becoming a quantitative tool for the study of surfaces to complement the well-established technique of low-energy electron diffraction (LEED). The change in the sign of the charge from e^- to e^+, the absence of an exchange term in the scattering Hamiltonian, and differences in correlation effects make the interactions of positrons with a surface significantly different from those of electrons. As there is no readily available means for producing large quantities of low-energy positrons, the development of a

e^+ beam of sufficient flux and collimation for diffraction studies is considerably more difficult than for electrons.

The development of slow e^+ beams made possible the first e^+-surface interaction investigations leading to the discovery of large positronium (Ps) formation cross sections.[2] This technique has more recently been applied in ultrahigh vacuum (UHV) permitting the study of e^+ interactions with well-characterized clean surfaces.[3] These measurements showed that even at a pure metal surface Ps formation is predominant, and have led to the study of Ps surface states as well as e^+ and Ps work functions.

Most e^+-beam experiments have been done with solenoidal magnetic transport systems which allow neither sufficient incident beam collimation nor, because of the strong magnetic fields, angular resolution of the scattered beams. Therefore, to investigate the feasibility of LEPD we have built an electrostatic positron transport system which was designed as a compromise between minimum energy, angular, and spatial beam spread and maximum beam transmission. Our apparatus consists of an UHV ($\lesssim 10^{-10}$ Torr) system equipped with an Auger spectrometer, an ion bombardment gun, and a quadrupole mass spectrometer. The transport system is shown in Fig. 1. Fast e^+ from the ^{58}Co source are converted to slow e^+, accelerated by the gun, focused through a parallel-plate analyzer by an einzel field lens and finally decelerated and focused onto the target by the zoom lens. Helmholtz coils are used to cancel the ambient magnetic fields. The converter consists of a 1-cm-diam arrangement of parallel, well-annealed tungsten ribbons[4] yielding 4×10^5 slow positrons per second for a 450-mCi source.[5] The emitted low-energy positrons have a characteristic energy spread of 3 eV full width at half maximum. The converter is placed at the cathode position of a low-energy gun based on an adaptation of a Soa immersion lens.[6] This gun is used to extract and accelerate the positrons to either 400 or 200 eV. The beam is then deflected 90° by a high-transmission, low-resolution parallel-plate analyzer to prevent the unconverted e^+ and γ products of the source from reaching the target. A glass insulator divides the system into a gun and a target region; the energy of the beam incident on the target (E) is the kinetic energy with which the positrons leave the gun region minus the potential difference between the gun and target regions. (The zoom lens allowed E to be varied from 0.1 to 1.0 times either of the two gun energies.) With the gun at 400 eV the system transmission ranged from 4% to 10% of the ($\approx 100\%$) transmission of a magnetic solenoidal system; with the gun at 200 eV the transmission was halved. The beam diameter and location were measured with a channel electron multiplier (CEM). The diameter of the beam was found to be 5.5 ± 1 mm over the full 20–400-eV range; the centroid of the beam stayed within 2 mm of the zoom-lens axis.

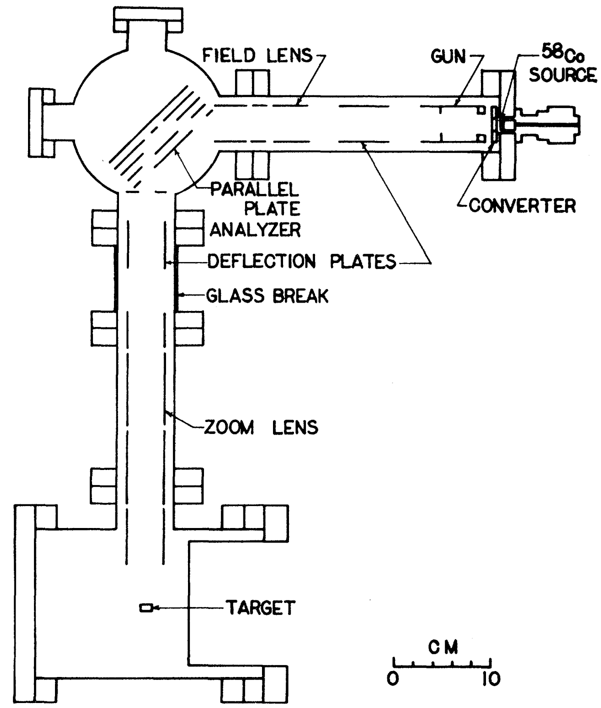

FIG. 1. Source, converter, and beam-transport system.

The scattering region is shown in Fig. 2. The incident beam impinges on the sample at an angle θ_i and is scattered at an angle θ, both measured with respect to the normal ($\vec{N}$) of the crystal surface plane. The detector consists of a retarding-field analyzer (RFA) in front of a CEM mounted on a goniometer. This moves in an arc in the scattering plane defined by $\vec{N}$ and the zoom-lens axis. The detector was 33 mm from the center of the sample with an effective aperture of 8 mm yielding a 14° acceptance angle. The NaI(Tl) detector monitored the positron-annihilation γ's and was used to measure the beam flux at the target and, in coincidence with the CEM, to confirm that the CEM was detecting positions. The magnetic field in this region was reduced

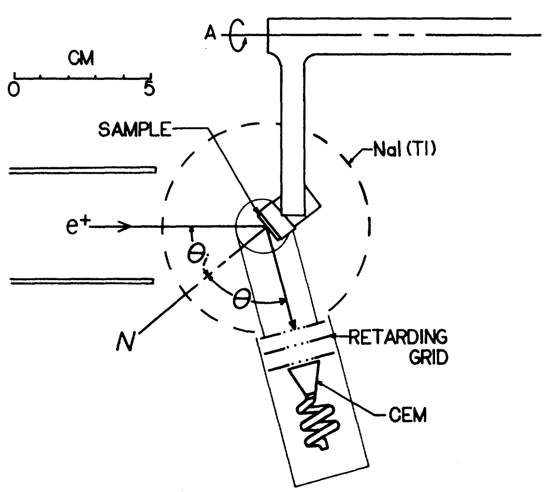

FIG. 2. Scattering region. The positron beam strikes the sample at θ_i with respect to the (111) surface normal $\vec{N}$. The channel electron multiplier (CEM) travels in a plane defined by the incident-beam direction and $\vec{N}$; θ is the scattering angle. The NaI(Tl) detector is placed 5 cm behind the sample. Rotation about axis A brings the sample to the focus of an Auger cylindrical-mirror analyzer (CMA) and an ion bombardment gun (neither shown).

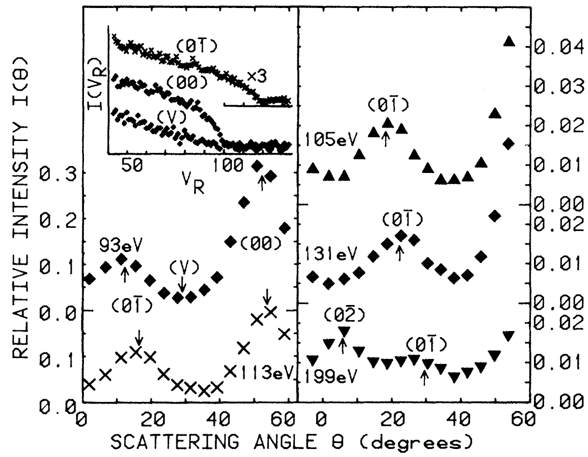

FIG. 3. Intensity of elastically scattered positrons vs angle and energy. Arrows point to the calculated diffraction angles. On the left the inset shows intensity vs detector retarding grid potential; the upper curve corresponds to the cited location on the 113 eV ($\theta_i = 54°$) plot, the lower two to the 93 eV ($\theta_i = 52°$). The motion of the diffraction peaks vs energy is shown on the right at 105 eV ($\theta_i = 58°$), 131 eV ($\theta_i = 60°$), and 199 eV ($\theta_i = 62°$).

to less than 30 mG thus having a negligible effect on the e^+ trajectories.

The Cu sample was cut from a 99.999%-pure boule oriented within 1° of the (111) face, annealed, and then mechanically polished. It was mounted in the sample chamber such that the projection of the incident-beam direction onto the crystal was within 3° of the $\langle 11\bar{2}\rangle$ direction (which is the direction we defined as the k_y axis of the reciprocal surface lattice). Cleaning consisted of several cycles of argon-ion sputtering followed by annealing. Contamination levels were determined with an Auger spectrometer; carbon at a small fraction of a monolayer, was the principal contaminant.[7]

The scattered positrons were counted with the CEM as a function of detector angle and incident energy at fixed sample angles; the count rates ranged as high as 70 s^{-1}. By sweeping the potential (V_R) on the RFA grid for fixed θ and E, we confirmed that the maxima which we attributed to diffraction peaks were due to elastically scattered positrons (inset, Fig. 3). We then set V_R at 10 V below the nominal beam energy to ensure maximum acceptance of the elastically scattered positrons while still rejecting the bulk of those inelastically scattered. Analysis of the specular-peak locations exhibited shifts from the predicted locations that could be attributed to increases in effective incident-beam angle with increasing incident energy. This shift, which may have been due to an insufficiently shielded lens element lead, is still under investigation. A quadratic fit of this shift with use of 27 specular peaks between 40 and 250 eV at θ_i(nominal) $= 48.5$ and 50° yielded a 10° shift in θ_i with a rms deviation of 1.4°. Using these fitted values of θ_i, we were able to predict the angular maxima in our ≈ 60 runs within 2° of the observed (00), $(0\bar{1})$, and $(0\bar{2})$ peaks. Figure 3 shows representative $I(\theta)$ spectra. The arrows point to the predicted locations of the peaks. We attribute the 16° full width at half maximum of the specular peak to the incident-beam spread (an estimated 5°) and the 14° detector acceptance angle. Spreading because of surface defects and thermal vibration is comparatively negligible. The relative intensities are estimates (in percent) of the scattered intensities.

In Fig. 4 we show an $I(E)$ curve recorded with the detector at $\theta = 34°$ over the 20–400-eV range. The energy scale has been calibrated according to $I(V_R)$ curves; contact-potential corrections, which are believed to be small, are neglected. The arrows are drawn at the calculated Bragg peaks with use of the bulk spacing with no inner-

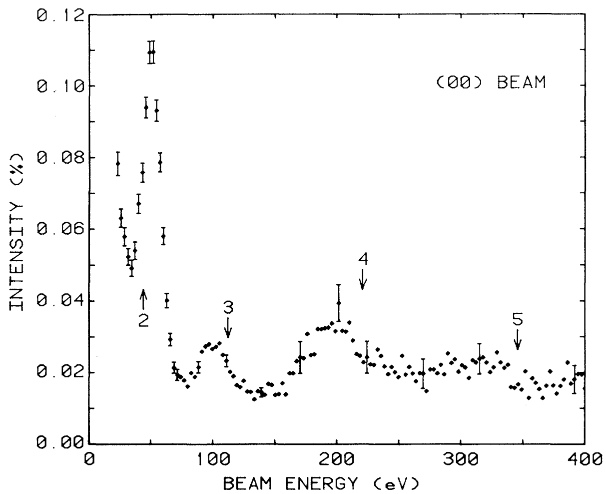

FIG. 4. $I(V)$ curve. The arrows point to the calculated locations of the primary Bragg peaks (no inner-potential correction). The data are a normalized sum of 20–150- and 40–400-eV runs. The intensity scale is based on the percentage of the incident beam detected.

potential corrections; the shift in θ_i is taken into account. θ_i varied from $\approx 27°$ to $\approx 38°$ over the energy range; the fraction of the beam detected was a maximum at ≈ 115 eV and fell off by 50% at 20 eV and 30% at 400. The intensity scale is calibrated for $E = 115$ eV. At this time we do not have theoretical predictions for the amplitudes or locations of the peaks; however, these calculations are in progress.

Although the diffracted intensities are weak, we have shown them to be sufficient to make LEPD measurements. We are working on improvements in beam design, such as the converter recently developed by Mills,[8] to obtain a higher-intensity, narrower-spread beam with which to make higher-precision measurements.

The similarities between e^+ and e^- make comparisons of LEPD and LEED valuable as a test for theoretical models of surfaces. Because e^+ in solids are not subject to Pauli exclusion, their mean free path between inelastic collisions should be shorter than that for e^- at particle energies $\lesssim 100$ eV.[9] This would affect the penetration depth and would also be important in studies of inelastic LEPD. As the e^+ from a ^{58}Co source are spin polarized and are not significantly depolarized while slowing down in matter,[10] our beam is probably polarized. This suggests studies of polarized LEPD similar to those now being made for polarized LEED.[11] As we continue to improve our beam we will be able to investigate these comparisons with LEED.

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