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Observation of elastic scattering of positrons and electrons at glancing incidence

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Elastic intensity versus energy (I-V) spectra have been observed using both positrons and electrons scattered at glancing incidence (83°–56° with respect to the surface normal) in the energy range of 50–450 eV from a variety of metallic and alkali-metal-halide surfaces. Unlike the electron spectra under the same conditions, all glancing-angle positron I-V spectra have broad (≥ 100 eV) features. The enhanced broadening is associated with the reduced penetration depth of the elastically scattered positrons. Peak positions and widths fit a quasikinematic calculation of the intensity for Cu(100).

The study of low-energy elastic scattering of positrons has provided new information about condensed-matter surfaces. Intensity versus energy (I-V) from low-energy-positron-diffraction (LEPD)[1-3] studies complements low-energy-electron-diffraction (LEED) work because the exchange interaction is absent and the contribution to the correlation energy from interactions with core electrons is diminished due to the repulsion of positrons from the ion cores. Such studies require a monoenergetic positron beam with high brightness (low angular spread, small diameter) due to the restrictions of large coherence length (>100 Å) and finite sample size. These elastic positron scattering studies have become feasible due to the implementation of the brightness-enhancement multiple remoderation technique of radioactive positron sources.[4] Recently,[5] analysis of a close comparative study of LEED and LEPD I-V spectra from six and seven nondegenerate diffraction beams, respectively, and incident beam polar angles of $\theta \approx 50°$, showed quantitative agreement between the two spectroscopies for the multilayer relaxation of a Cu(100) surface and confirmed the validity of the potentials and the need for a multiple scattering analysis in the computation.

At typical LEED energies, the glancing-angle geometry emphasizes the differences in positron versus electron scattering that are not as readily evident in normal-incidence spectra. Since the surface normal component of the beam energy $E_\perp = E\cos^2\theta$ is low (of order 10 eV), the detailed form of the electron and positron surface scattering potentials (the real, V_{0r}, and imaginary, V_{0i}, components of the positron inner potential) strongly affect the scattering spectra. The relatively repulsive nature of the positron inner potential (V_{0r}) compared to the attractive electron inner potential should reduce positron penetration of the bulk, thus enhancing reflection. In fact, it has been suggested[6] that total reflection of high-energy (≈ 30 keV) positrons scattering at glancing incidence off the repulsive inner potential barrier may provide a direct measurement of the surface dipole potential D. The presence of strong inelastic scattering for positrons implies that multiple scattering is strongly attenuated at low values of $E_\perp$ and the positron scattering can be understood by invoking kinematic rather than the dynamic models which explain the high-$E_\perp$ data.

The present work is a comparative study of elastically scattered beams of electrons and positrons at glancing angles (polar angle $\theta \leq 83°$ with respect to the surface normal) and beam energy $E = 50$–450 eV off a variety of surfaces, namely, W(110), Cu(100), Cu(100) plus oxygen in the ordered superlattice $\sqrt{2}\times 2\sqrt{2}\,R45$, Al(110), Ni(110), LiF(100), and NaF(100). This experimental study finds the glancing-angle positron specular I-V spectra to have peaks (at the Bragg energy and lower than the $n=1$ Bragg energy) with anomalously large widths (>100 eV) for all samples. On the other hand, glancing-incidence electron I-V spectra are found to have narrow peaks under comparable conditions and good agreement exists between the experimental data and calculated spectra generated from the standard model[7] (see Ref. 8 for a similar study of electrons). This work suggests that the enhanced energy width in the positron data is due to the diminished penetration depths of positrons relative to electrons for the targets studied. Although the multiple scattering model successfully describes this positron I-V spectra for an incident beam angle lying closer to the surface normal ($\approx 50°$), a quasikinematical model is more suitable for glancing incidence conditions.

An earlier publication[4] described and listed the characteristics of the doubly remoderated electrostatic positron beam. The source end of the beam has been subsequently modified by inserting a ^{22}Na positron source and thin (≈ 1 μm) transmission W(100) moderator.[9] The elastically scattered positrons are detected with a position-sensitive detector.[4] A previous publication[5] described the procedure for determining the incident beam angle to an accuracy of $\pm 0.8°$. All the samples are pure ($>99.999\%$) and well oriented [$\leq 1°$, except Al(110) and W(110) which are oriented to within 2°]. The metal samples [except W(110)] are cleaned using the standard cyclic 1000-V argon sputter and anneal procedure. To remove carbon impurities from the surface, the W sample was cyclically heated to ≈ 1300 °C and exposed to 1000 L (1 L$=10^{-6}$torr sec) oxygen at ≈ 1000 °C. The polished LiF(100) was cleaned in UHV ($<1\times10^{-10}$ torr) by heating to 300 °C. Impurities were removed from the NaF sample by exposing the heated sample to low-energy (60 eV) electrons for a few minutes from a commercial Varian LEED system and rastering the beam over the sample. A sharp LEED pattern eventually appeared during the exposure. Such a procedure had the virtue of monitoring the surface condition without inducing damage to the sample. Surface charging of the alkali-metal-halide crystals was eliminated by heating the sample to ≈ 200 °C.

The normalized (to the incident beam rate) experimental glancing incidence *I-V* spectra for positrons and electrons were observed[10] from W(110), Al(110), LiF(100), Ni(110), and NaF(100) targets; spectra from the latter two are shown in Fig. 1. The positron spectra have only broad features for the Bragg peaks and peaks which occur at an energy less than the first Bragg peak.[10] The expected position of the nth-order Bragg peaks using the simple kinematic description, the known interlayer spacing, and inner potential are labeled with an arrow in Fig. 1.

The peak widths of the positron *I-V* spectra (for specular and nonspecular beams) are monotonically increasing functions of the polar beam angle but only weakly dependent on the perpendicular component of energy $E_\perp = E\cos^2\theta$ [see Figs. 2 and 3(a)]. In Figs. 2 and 3(a), the normalized specular LEPD are plotted as a function of $E_\perp$ for a variety of polar angles. The peak intensities in Fig. 2 have been rescaled to a common value. The mismatch of $E_\perp$ for the experimental peaks in Fig. 2 are consistent with an experimental polar angle error of $\approx 0.8°$. The widths of the electron data are relatively independent of the incident beam angle. The position of the maximum of the peak intensity in the positron *I-V* curve agrees with the functional dependence on incident polar angle predicted from kinematic Bragg scattering. As the sample temperature is raised, the peak intensities of the positron spectrum are diminished. In the present experiment, part of the data is such that the perpendicular energy $E_\perp = E\cos^2\theta$ is less than D and the beam energy E is high, so that the attractive correlation potential is predicted to diminish. Under these conditions, Oliva[6] suggested that in the absence of inelastic processes, positrons should reflect from the metallic surface with a large probability and a sudden increase in the reflectivity should occur when $E_\perp \leq D$. Evidently, inelastic effects at these relatively low energies (50 to 450 eV) broaden the barrier and prevent the observation of positrons reflecting off the dipole layer [see Fig. 3(a) and Ref. 11 for D].

The broad features in the positron spectra can be explained as due to the reduced penetration of the elastically scattered positrons into the target materials which becomes smaller than the layer or atom separation (<1 Å). In the case of positrons, there exist inelastic scattering channels that are not available for electrons, such as annihilation and fast positronium formation at glancing angles;[12] also inelastic collision rates are reduced for elec-

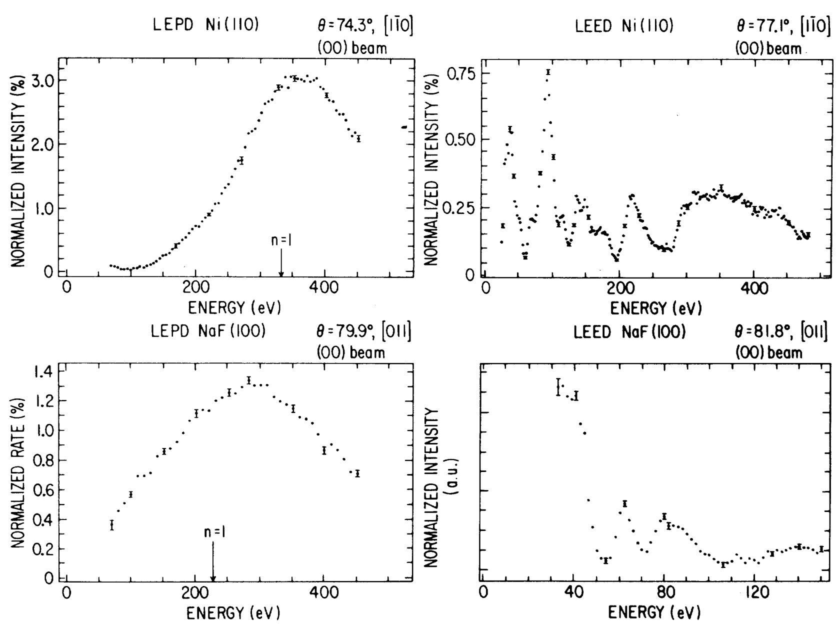

FIG. 1. Comparison of normalized specular LEPD and LEED spectra from NaF(100) and Ni(110). The arrow below $n=1$ denotes the first-order Bragg peak position.

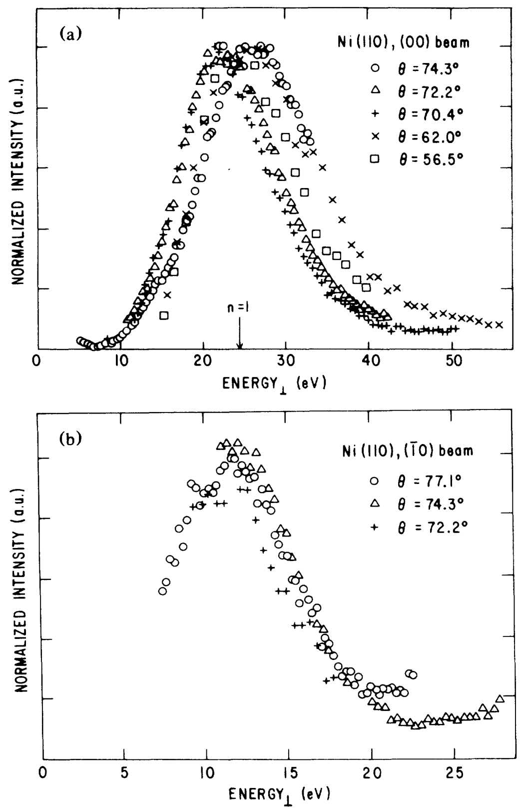

FIG. 2. (a) Normalized specular LEPD from Ni(110) plotted as a function of $E_\perp$ (projected energy along surface normal) for various incident polar angles as denoted in the figure. All intensities rescaled to a common peak value. First-order Bragg peak denoted by arrow. (b) Similar plot for ($\bar{1}$,0) beam.

trons due to the "Z^3 effect."[13] These scattering processes attenuate the elastic beam and diminish the penetration depth for the positron beam. Electron-hole and plasmon formation by positrons and electrons have similar cross sections at these energies[14] and therefore do not explain the qualitative differences in the spectra. In conventional LEED *I-V* formalism, the strength of the inelastic processes is given by the imaginary part of the inner potential V_{0i} which is predicted to have an energy dependence. Earlier work on Cu(100) (Ref. 5) indicated that indeed the imaginary part of the positron inner potential (−6 eV) exceeds the value for electrons (−4 eV) and there are large differences in the real part of the inner potential V_{0r},[5] which is strongly attractive for electrons (−11 eV in Cu) relative to positrons (0 eV in Cu).

Unlike the spectra from electron scattering, earlier results for the peak positions in the normal-incidence low-energy ($n=1$ Bragg peak) position spectra *I-V* studies[15,16] were explained by using the kinematic model and assigning the real part of the inner potential to the positron work function of the material. In the present work, it is suggested that inelastic scattering for positrons exceeds the elastic scattering cross section and therefore the broad features and enhanced reflection in glancing incidence positron scattering can be reproduced by a quasikinematical model. The calculations are shown in Fig. 3(b) for copper. In such a model, the appropriate real and imaginary parts of the inner potential are used for the potential between atoms and only single atom scattering is considered. The scattering from the atom is treated exactly. The atomic form factor is found by solving the Schrödinger equation with a potential that contains the Coulomb interaction (opposite in sign to the electron potential) and no exchange, but retains the correlation interaction.

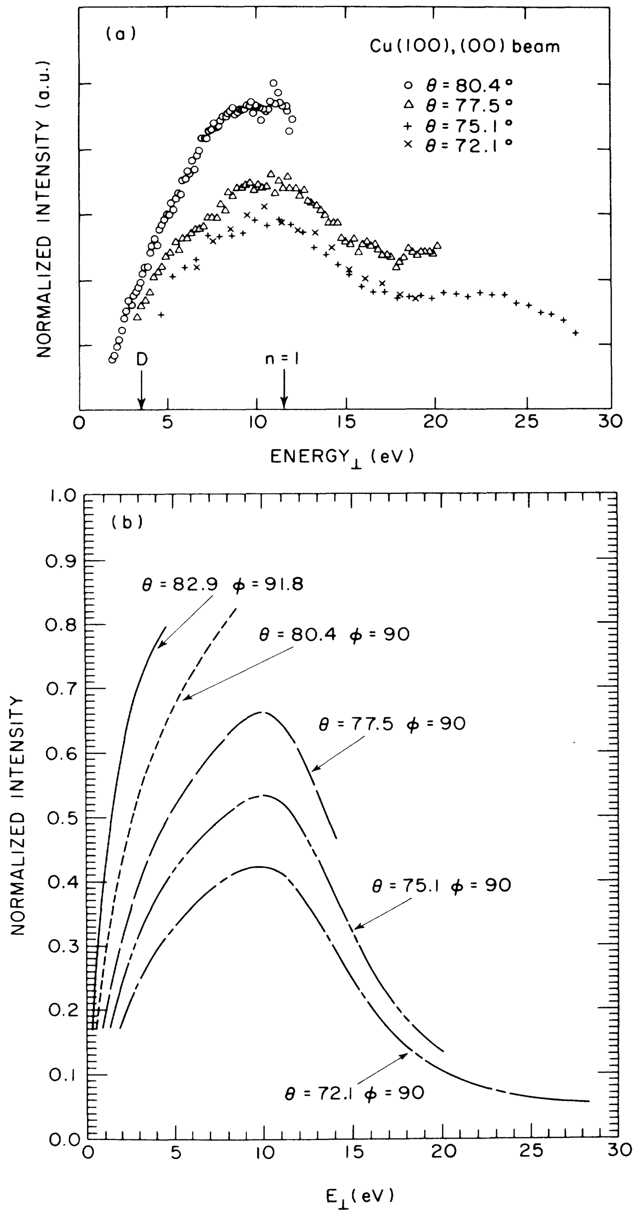

FIG. 3. (a) Experimentally observed normalized specular LEPD from Cu(100) for various polar beam angles as denoted in the figure. First-order Bragg peak indicated by arrow below $n=1$ and position of dipole potential D is also displayed. (b) Calculated specular LEPD from Cu(100) for various polar beam angles using the quasikinematic model.

In addition, the predicted penetration depths λ_z ($1/e$ distance for intensity attenuation) into the attenuating medium from the quasikinematic model are plotted against polar angle θ in Fig. 4 where

$$\lambda_z = 1.95 \frac{(E_\perp - V_{0r})^{1/2}}{-V_{0i}} \quad (\lambda_z \text{ in Å}; E_\perp, V_{0r}, V_{0i} \text{ in eV})$$

approximately. The calculated penetration depth is reduced at glancing angles with a limit at 90° of ≈ 0.55 Å for all energies on copper. At higher energies, multiple scattering plays a larger role and the kinematic picture is not adequate, as can be seen in the unusual peak shapes and energy mismatch with Bragg scattering,[2,3,5] [and Fig. 3(a)] due to the greater penetration of the positron under such conditions.

Values for V_{0i} were not extracted for the other materials. Nevertheless, penetration depths for the other samples can be estimated by using the following line of reasoning. Arguing analogously from optical diffraction,[15] there is a spread in the wave vector projected along the direction normal to the surface due to scattering off N diffraction layers of separation d. The average penetration depth Nd, is therefore given in terms of the projected energy $E_\perp$ of the $n=1$ Bragg peak in the I-V spectra and projected energy width $\Delta E_\perp$ along the surface normal by the expression

$$Nd = \frac{h}{2\Delta E_\perp} \frac{\sqrt{E_\perp}}{2m} .$$

Applying these ideas to the experimental I-V spectra, the derived penetration depths for positrons for a variety of materials are 1–2 Å. Electrons under comparable conditions have penetration depths of order 6 Å.[17]

In summary, we have observed and noted the behavior of positrons as they elastically scatter at glancing angles and how their behavior differs from that of electrons. Under the present experimental conditions, the intensity of the diffracted beam cannot be explained by the reflectance from the surface dipole potential. Shallow penetration explains the broad features in the positron spectra. Development of a more exact theory and detailed calculations are needed to establish the energy dependence of the elastic and inelastic cross sections for positrons. Finally, diminished penetration and absence of multiple scattering may provide a new structural tool for position measurement of adsorbates on substrates and determination of surface roughness.

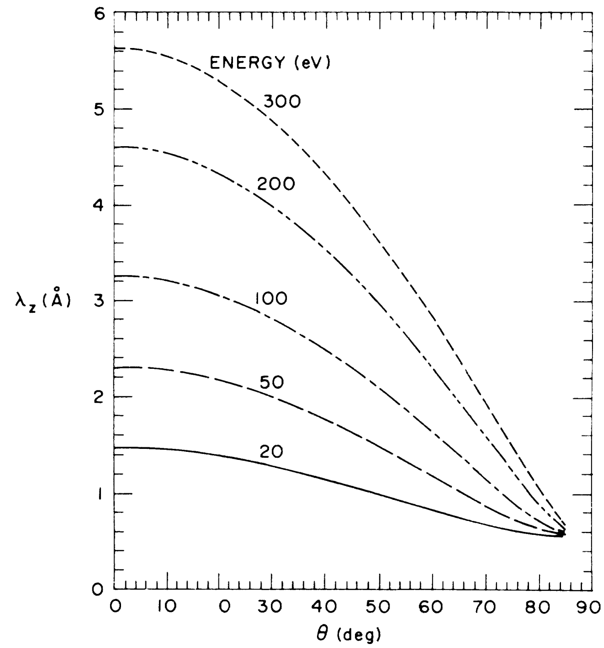

FIG. 4. Calculated positron penetration depths λ_z vs polar angle θ for various energies (eV). Sample is Cu(100).

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