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Test of the Electronic Structure of Fe(100) by Absorbed Current Spectroscopy

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Abstract

The absorbed electron current for a clean Fe(100) surface as a function of energy rises step-like at the vacuum-energy cutoff with an absorption close to 1. The smooth decrease of absorbed current at higher electron energy due to secondary electron emission is superimposed by a considerable amount of fine structure, the amplitude of which decreases with increasing energy. These features are found in good agreement with the results of a calculation of the elastic part of the electron reflection coefficient. Further, they are compared with the ferromagnetic electronic bulk bandstructure calculated above the vacuum energy. From the comparison with the experimental data, the energy dependence of the real and imaginary parts of the inner potential is determined.

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1. Introduction

The electronic quasi-particle spectrum of metals below the Fermi energy E_F is well known from photoemission experiments. Much less information is as yet available on the electron states well above E_F. These states do not show up directly as peaks in photoelectron energy distribution curves (EDC's), but they are, as final states, important for the identification of the initial states in photoemission and their lifetime contributes to the peak width in the photoemission EDC. It is therefore desirable to obtain reliable first-hand information on the energy levels of these higher states and on their lifetimes. It is shown in this work that a method to determine the electronic structure at higher energies with high accuracy is to measure the electron current I(E) absorbed by a clean single-crystal surface (target current) as a function of the primary electron energy.

The absorbed electron current can be written as $I = I_o$(1-R), where I_o is the primary current and R is the total reflectivity. R consists of two terms, an elastic contribution R_e, and an inelastic part R_i. R_e is the usual low-energy electron diffraction (LEED) reflectivity and is calculated within the framework of a dynamical LEED theory(1). Since R_e has a (local) maximum when the electron energy falls in a bandgap of the quasi-particle bandstructure, it is to be expected that the absorbed current as a function of energy is modulated in correlation with the bandstructure. Furthermore, due to the spin dependence of the bandstructure and of the absorptive potential of ferromagnets, spin-dependent effects are to be expected, which will be explored in future studies(2).

2. Apparatus

We made use of the surface analysis facility at SLAC(3), which provided the ultrahigh-vacuum surrounding and surface analysis facilities for the present experiment. The pressure was in the low 10^{-10} Torr range, and the sample could be cleaned by ion etching and heating. Surface conditions have been determined by LEED and Auger-spectroscopy. The sample was a thin disk of high-purity Fe(100), polished mechanically and chemically, and cleaned in-situ by repeated ion etching and heating. It was mounted to a Nb sample holder. Prior to insertion into the vacuum chamber it had been demagnetized. The sample was also heated to 1.04 times the Curie temperature in vacuo several times. When performing the absorbed current measurements, the sample was transferred to a magnetically shielded region ($B_o \sim 1mG$), which also covered the electron gun. For enabling measurements at different polar angles of incidence, the sample was attached to a rotary feedthrough. To avoid charging effects at low energies, it was found necessary to plate the surfaces surrounding the sample by a layer of gold.

The electron current was provided by a five-electrode electron gun with an oriented single crystal LaB_6 rod cathode (Fig. 1). By means of x-y deflection plates the beam could be scanned across the sample and its holder, and an image was produced on a TV monitor. This enabled us to estimate the width of the electron beam as a function of incident energy, and by choosing suitable operation conditions of the gun, a virtually constant beam size at the sample could be obtained between 2 and 100 eV electron energy. By electron ray tracing, employing the "Charged Particle Ray Simulator and Monitor"(4), it was determined that no intermediate focusing occured in this energy range. The target current was measured with an analog electrometer coupled (via an A/D converter) to a computer operating in multipass averaging mode. The electron energy was ramped by applying a ramp voltage to the cathode and the first three lens elements. Data of about 100 runs were accumulated.

3. Experimental Results

In Fig. 2a, the target current to the Fe(100) sample is shown for normal incidence, normalized to the primary current. It is observed that the current reaches its maximum value within an energy range corresponding to the energy width of the electron beam (0.3 eV). The relative absorption is close to 1. It then decays smoothly until it crosses through zero (not shown) at about 110 eV. The smooth decrease of absorbed current is interpreted as resulting from the increase in escape cone for inelastically scattered electrons. Superimposed are small structures which are enhanced in Fig. 2b by calculating the second derivative. This procedure also eliminates the smoothly varying background. The smoothed second derivative is obtained from a cubic spline fit(5) to the data. Further details and data obtained at other angle of incidence will be published elsewhere(7).

4. Theoretical Interpretation

The target current (normalized to the primary current) can be expressed as

$$I(E) = 1 - R_e(E) - R_i(E), \tag{1}$$

where R_e and R_i are the elastic and the inelastic reflection coefficients, respectively. Since R_i is a comparatively slowly varying function of energy, we focus on R_e(E), which is the sum of the intensities of the LEED beams leaving the surface at energy E. As is well known, the energetic positions of structures in R_e(E) depend – for given surface geometry and ion-core potential – mainly on the real part V_r(E) of the inner potential, while their width is determined by the absorptive potential V_i(E). Comparison with experimental target current data therefore provides information on these potential contributions.

We have performed dynamical LEED calculations(1) for Fe(100), assuming the real inner potential as $V_r(E) = 14.5exp(-E/E_o)$ (eV) with $E_o = 350.9$ eV(6) and the imaginary potential as a preliminary form covering the energy range between the vacuum level and about 60 eV above it as $V_i(E) = 0.7 + \alpha E$ eV with $\alpha = 0.044$. The second derivative $-R_e''$(E), which should (cf. eq. (1)) be the dominant factor for the target current second derivative I''(E), was calculated from the theoretical R_e(E) values by employing the spline fit routine(5) with the same parameters as were used for the experimental data. The bulk bandstructure (above vacuum level) was calculated using the same real potential as in the LEED calculation.

Theoretical results for (1-R_e) and its second derivative are shown in Fig. 2c. It is seen that the fine structures agree well between theory and experiment, and also the amplitude ratios are qualitatively reproduced. The close fit of the experimental $I''(E)$ with the theoretical $-R_e''(E)$ results indicates that inelastic processes do indeed not produce significant structures. By comparing with the calculated bandstructure along Γ - H (Fig. 2d), it is concluded that the features can all be regarded as band-structure effects. The theoretical interpretation will be given in more detail elsewhere(7). The minima in the second derivative correspond to maxima in the absorbed current. They do not occur at the maximum density of states since there the group velocity is zero, but shifted slightly away from the band edges into the bands. This kind of correlation has recently also been found in angle-resolved secondary electron emission from Cu(100)(8). LEED beam emergence thresholds are observed weakly as structures around 18 and 35 eV in the calculation, but they are also much weaker than the features associated with the bandstructure.

5. Conclusion

The absorbed electron current to the Fe(100) surface as a function of energy displays a significant amount of structures which is closely related to the bulk bandstructure above the vacuum level. Good agreement exists with the elastic reflection coefficient calculated by dynamical LEED theory. The low-energy part of the I(E) curve contains information on the surface potential barrier, which still is the subject of further investigation.

6. References

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7. Figure Captions

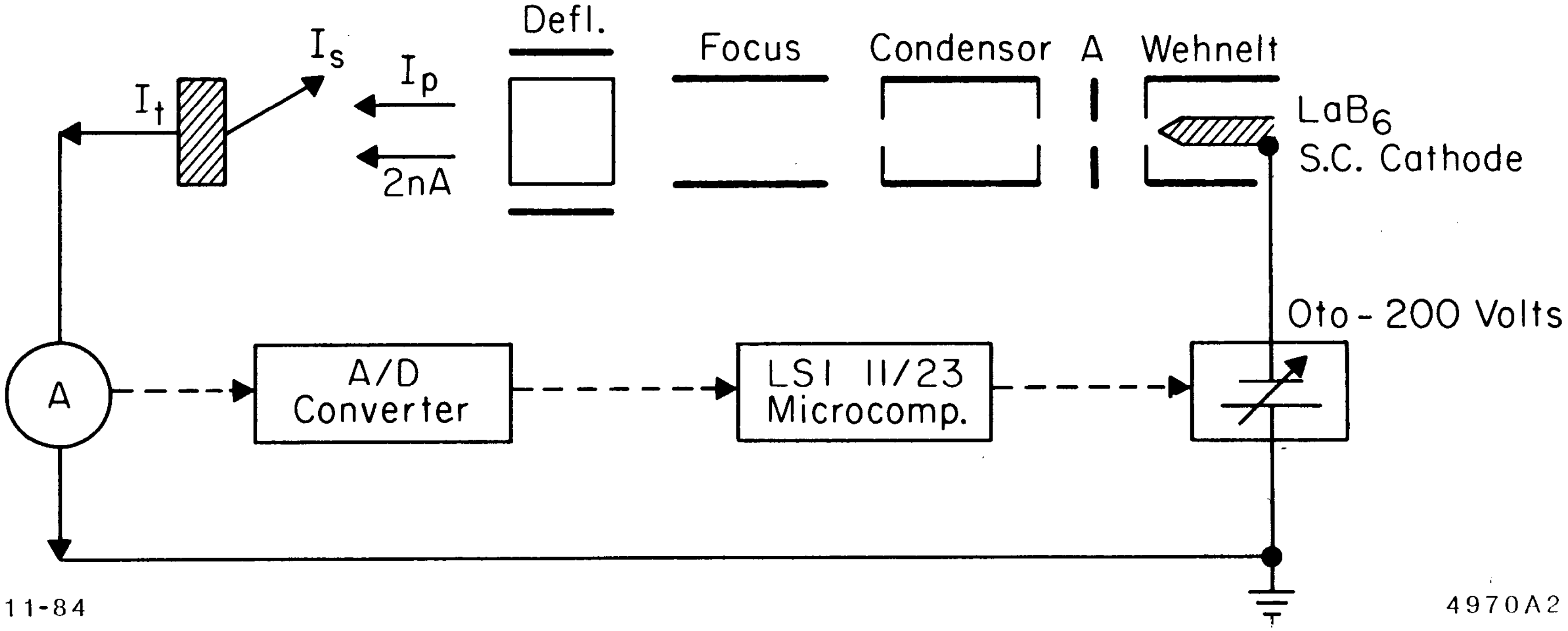
1 Experimental arrangement

2a Normalized absorbed current I(E) for electrons normally incident on an Fe(100) surface (energy E relative to the vacuum zero).

2b Smoothed second derivative of the absorbed current (arbitrary units).

2c Spin-averaged theoretical results for $1 - R_e(\mathrm{E})$ (- - -) and $-d^2R_e(E)/dE^2$ (—, arbitrary units), where R_e is the elastic reflectivity.

2d Bulk bandstructure of Fe along the Γ - H direction.

Defl.
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I_p
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A
A/D Converter
LSI 11/23 Microcomp.
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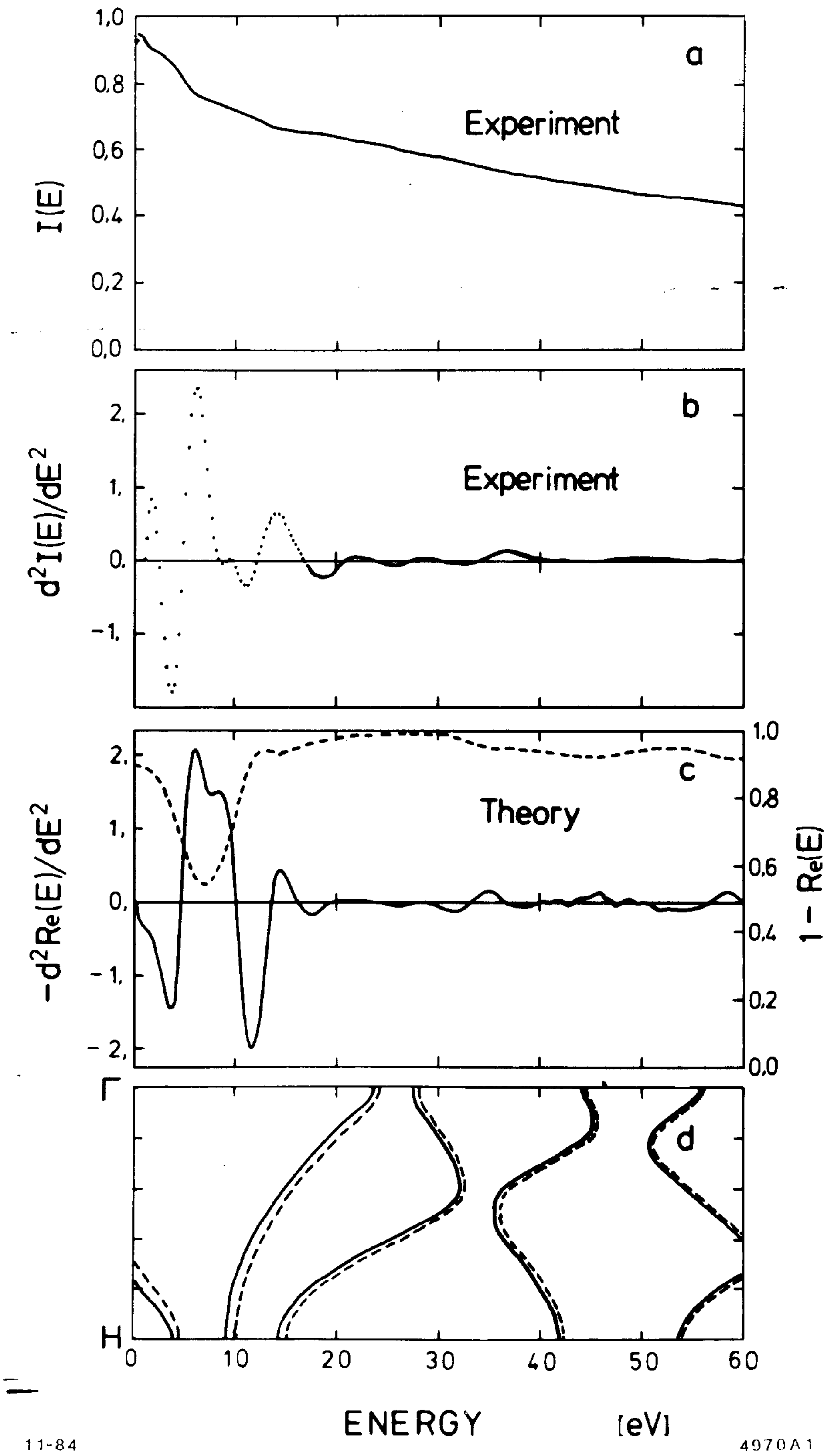
Fig. 1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0,8
0,6
0,4
0,2
0,0
I(E)
a
Experiment
2.
1.
0.
−1.
$d^2I(E)/dE^2$
b
Experiment
2.
1.
0.
−1.
−2.
$-d^2Re(E)/dE^2$
c
Theory
1.0
0,8
0,6
0,4
0,2
0,0
1 − Re(E)
Γ
H
d
0
10
20
30
40
50
60
ENERGY
[eV]
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Fig. 2