Solid State Communications, Vol. 84, No. 5, pp. 541–544, 1992.
Printed in Great Britain.

0038–1098/92 $5.00 + .00
Pergamon Press Ltd

SPIN-DEPENDENT ELECTRON REFLECTION FROM Fe(1 1 0): EXPERIMENT AND THEORY

G. Fahsold, M.S. Hammond and J. Kirschner*

Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, D-1000 Berlin 33, FRG

and

J.W. Krewer and R. Feder

Universität Duisburg, Theoret. Festkörperphysik, W-4100 Duisburg, FRG

(*Received* 25 *June* 1992 *by M. Cardona*)

For spin-polarized low-energy (0–50 eV) electrons incident on magnetized Fe(1 1 0) we have measured and dynamically calculated the elastic reflected current and the exchange-induced scattering asymmetry associated with it. The structure of the asymmetry is related to the spin-split band structure above the vacuum level. A large asymmetry peak around 5 eV, where the current is also large, is very stable against changes of the incidence angle and variations of the potential and the surface magnetization. This suggests a very efficient spin polarimeter.

1. INTRODUCTION

THE APPLICATION of electron reflection [1] and absorption [2–4] measurements to the identification of major features in the unoccupied electronic band structure of solids has long been established. As an extension of these measurements to ferromagnetic materials, Tamura *et al.* [5] suggested measuring the spin-dependence of low-energy electron absorption or reflection and went on to calculate the dependence of the elastically reflected current on the spin orientation (relative to the sample magnetization) of a polarized electron beam incident on a Fe(0 0 1) surface. Recently, comprehensive measurements of the normalized difference in the absorbed or reflected current for incident electron spin parallel and antiparallel to the sample magnetization have been made on Fe(1 1 0) [6, 7]. These difference (or "spin asymmetry") measurements have demonstrated the importance of the spin-split bulk band structure for the spin-dependent transmission and reflection of electrons at energies up to 50 eV.

We report here the first comparison of calculated elastic electron reflection spin asymmetries to experiment. We find good agreement between experiment and theory, and demonstrate the advantages that a spin-polarized electron reflection measurement has over its spin-averaged counterpart for unambiguously identifying manifestations from electronic bulk and surface structure. In Sections 2 and 3 the experimental and theoretical methods employed are briefly outlined. The results are discussed in Section 4 and a description of how certain elastic scattering effects from iron may be used in an electron spin-polarization detector is also included.

2. EXPERIMENT

The apparatus used to measure the elastic reflected current spin asymmetries has been described in detail elsewhere [6]. In short, a spin-polarized primary electron beam (polarization $P_0 \approx 20–30\%$ and energy $E_0 = 0–50\,\mathrm{eV}$) is focussed through the center of a 3-grid hemispherical LEED analyzer. The 3-grid LEED analyzer is used as a retarding field energy analyzer for the reflected electrons, with the second grid properly biased to reject inelastically scattered electrons and the third grid used as a collector. For the data presented here, the retarding voltage on the second grid was chosen such that electrons suffering less than 1.5 eV energy-loss were accepted. While the sample is connected to ground the first grid is held at constant potential to compensate the electric field between the sample and the LEED optics due to unequal work functions. The primary electrons are incident upon the (1 1 0) face of an iron single crystal in the (0 0 1) plane at an angle of 15° from normal incidence. The incident electron

---

* Permanent address: Max-Planck-Institut für Mikrostruturphysik, Weinberg 2, 0-4050 Halle/Saale, FRG.

spin-polarization is either parallel or anti-parallel to the remanent sample magnetization along the ⟨0 0 1⟩ direction. The reversal of the incident electron polarization at a frequency of 1 kHz allowed the use of a lock-in technique to detect the dependence of the elastic reflected current on primary electron polarization. The measured spin asymmetry $A(E_0)$ is thus defined as

$$A(E_0) = \frac{1}{|P_0|}\,\frac{I^{\uparrow} - I^{\downarrow}}{I^{\uparrow} + I^{\downarrow}}, \qquad (1)$$

where $I^{\uparrow}(I^{\downarrow})$ is the quasi-elastically reflected current with incident electron spin polarization P_0 parallel (anti-parallel) to the majority electron spin in the sample.

3. THEORY

Calculations were done with a relativistic layer-KKR formalism for ferromagnets (cf. [8] and references therein), which was recently extended – beyond the usual muffin-tin approximation – to allow for non-spherical effective potentials and magnetic fields in spheres around the lattice sites [9].

For the potential input we took, in addition to a conventional bulk form, results from a recent self-consistent full-potential linear augmented plane-wave (FLAPW) calculation (using the Barth–Hedin exchange-correlation approximation [10]) for a five-layer slab of Fe(1 1 0) [11]. The corresponding magnetic moments per atom are $2.6\mu_B$ for the surface layer and $2.32\mu_B$ for the central layer, as compared to about $2.2\mu_B$ from self-consistent bulk calculations (e.g., $2.18\mu_B$ from [12]). The real and imaginary parts of the inner potential were chosen as the energy-dependent forms deduced in [5]. The real part of the surface potential barrier was taken as continuous with image asymptotic behaviour as suggested in [13]. Its imaginary part was assumed as a Gaussian.

The elastic reflected current was calculated as the sum of the intensities of all elastically reflected beams. For the exchange-induced asymmetry we took, in accordance with the experimental procedure, the normalized difference of the currents for the primary-beam polarization parallel and antiparallel to the sample spin orientation, averaged over two opposite sample magnetization directions. For Fe, this quantity (labelled A_{ex} on p. 169 of [8]) is only very weakly affected by spin–orbit coupling and thus a very good approximation to the true A_{ex} (cf. [8], p. 170).

4. RESULTS

The measured and calculated spin asymmetries of elastically reflected current and the related spin averaged currents for electrons incident at 15° from normal as a function of primary energy are displayed together in Fig. 1. We see generally good agreement between the asymmetries [Fig. 1(b)] from experiment and theory, in particular with respect to the relative magnitude of the major features around 5 eV and 30 eV, the existence and energetic positions of zero-crossings (around 25, 35, and 45 eV), as well as the overall shape of the features between 5 and 15 eV and between 25 and 40 eV. We note that, to make contact with the measurements, the calculated spin-dependent intensities and consequently the asymmetry and the spin-averaged intensity [Fig. 1(a)] have been broadened by a Gaussian of width 0.5 eV. Thus, fine structure features associated with the emergence of LEED beams are washed out. But, as the figure shows, there is still one significant deviation of experiment from theory: the measured absolute asymmetry peak values are only about half of the calculated ones. This is most probably due to a combination of several effects: (i) insufficient energy resolution of the primary beam (approximately 0.5 eV), (ii) the angular integration of the measured reflected current (in the experiment the diffuse elastic background intensity is induced, while not in theory), and (iii) the collection of a finite amount of inelastically reflected electrons (recall that the retarding field analyzer is operated to collect electrons suffering less than 1.5 eV energy-loss).

If the surface layer potential from [11] is replaced by the central layer potential, the calculated

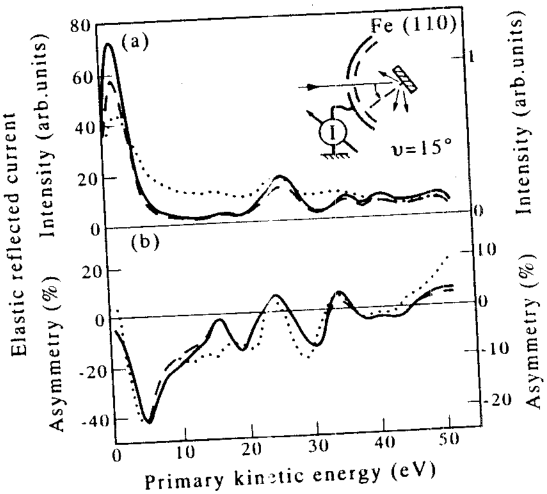

Fig. 1. Elastic reflected current from Fe(1 1 0) for polarized electrons incident on Fe(1 1 0) at polar angle 15°: (a) spin-averaged intensity, (b) exchange-induced scattering asymmetry. Experiment (dotted lines, right hand scale) and theory (left hand scale) for surface magnetization enhanced according to Ref. [11] (full lines) and bulk-like (dashed lines).

asymmetry is seen to change around 9 eV and in the peak at 33 eV, the latter agreeing better with experiment for the surface layer potential, which is associated with a 10% enhanced magnetic moment. More surprisingly, the intensity spectrum for the surface layer potential shows an overall enhancement by about 25%. We attribute this not to the enhanced moment as such, but rather to the different radial shape of the spin-split potentials, which have a larger jump at the atomic sphere radius (for details see Fig. 1 of [9]).

The peaks in the reflected current [Fig. 1(a)] are correlated with gaps in the quasiparticle energy band structure of the bulk and the asymmetry [Fig. 1(b)] directly reflects the exchange splitting of this band structure. This is similar to the observations used earlier for the target current [5]. In the reflected current, however, features can be identified directly, without recourse to taking first and second derivatives of the data such as done in [5]. Measurements and calculations for further angles of incidence, between 9 and 19 degrees incidence, show essentially similar results, with the same quality of agreement between theory and experiment.

In particular, around 5 eV there is always a large asymmetry peak associated with a fairly high intensity. This peak recommends itself as a particularly useful working point for an electron spin polarization detector. Earlier experiments [6, 7] have shown that, in this energy range, the asymmetry does not decrease in magnitude if the total reflected current is measured. This eliminates the need for energy discrimination of the reflected electrons, and therefore makes the realization of such a detector even simpler. Since the figure of merit F_m of a spin polarimeter [14] is typically defined as

$$F_m = \frac{I}{I_0} A^2,$$

where I_0 is the current into the detector (here: primary current), I is the measured current (here: reflected current) and A is the measured asymmetry. Collecting the total (energy-integrated) current without a loss of asymmetry results in an increase in the efficiency of this detector. At the low energies proposed for this polarimeter, the fraction of incident electrons that are reflected is 20%. Thus the figure of merit of the proposed detector would be approximately 8×10^{-3}. This exceeds a recent spin detector based on reflection from a Fe(0 0 1) surface [15] by about a factor of two and is more than an order of magnitude better than earlier spin detectors (cf. Refs. [16, 17]). Further advantages of the present detector are the following. Additional measurements [6] show that the reflected spin asymmetry for primary energies between 5 and 10 eV is rather insensitive to the angle of incidence around 15° within a range of ±4°. Furthermore, the collection of the angle integrated reflected current, in marked contrast to most existing spin polarimeters, increases the insensitivity to improper alignment. Calculations reveal that this asymmetry peak does not respond to changes (by about ±20%) of the surface magnetization. Some reduction of the latter, e.g. by contamination of the surface, should, therefore, not affect the operation of the detector. In our experiments the exposure to 2L oxygen resulted in a reduction of the asymmetry peak value from 20% to 19%, while the reflected current remained unchanged.

5. CONCLUSIONS

The intensity and the exchange-induced scattering asymmetry of the elastic low-energy electron reflection current from a magnetic Fe(1 1 0) surface have been obtained in good agreement experimentally and theoretically. Below 10 eV, a strong asymmetry feature occurs together with strong intensity, which seems very suitable for a highly efficient spin polarization detector. Further advantages of this proposed polarimeter are its insensitivity against moderate changes of the angle of incidence and against some reduction of the surface magnetization.

REFERENCES

1. E.N. Sickafus, *Phys. Rev.* **B16**, 1436, 1448 (1977).
2. R.C. Jaklevic & L.C. Davies, *Phys. Rev.* **B26**, 5391 (1982).
3. S.A. Lindgren, L. Wallden, J. Rundgren & P. Westrin, *Phys. Rev.* **B29**, 576 (1984).
4. S.A. Komolov & L.T. Chadderton, *Surf. Sci.* **90**, 359 (1979).
5. E. Tamura, R. Feder, J. Krewer, R.E. Kirby, E. Kisker, E.L. Garwin & F.K. King, *Solid State Commun.* **55**, 543 (1985).
6. M.S. Hammond, G. Fahsold & J. Kirschner, *Phys. Rev.* **B45**, 6131 (1992).
7. M.S. Hammond, G. Fahsold, K. Koike & J. Kirschner, *Vacuum* **41**, 500 (1990).
8. R. Feder, in *Polarized Electrons in Surface Physics* (Edited by R. Feder) World Scientific, Singapore (1985).
9. J.W. Krewer & R. Feder, *Physica B* **172**, 135 (1991).
10. U. von Barth & L. Hedin, *J. Phys.* **C5**, 1629 (1972).
11. J. Noffke, Private communication.
12. D. Glötzel, Private communication.
13. R.O. Jones, P.J. Jennings & O. Jepsen, *Phys. Rev.* **B29**, 6474 (1984).

14. J. Kessler, *Polarized Electrons*. Springer, Berlin (1976).
15. D. Tillmann, R. Thiel & E. Kisker, *Z. Phys.* **B77**, 1 (1989).
16. J. Kirschner, *Polarized Electrons at Surfaces*. Springer Tracts in Modern Physics, Vol. 106, Springer, Berlin (1985).
17. D.T. Pierce, R.J. Celotta, M.H. Kelley & J. Unguris, *Nucl. Instrum. Meth.* **A266**, 550 (1988).