Spin-dependent low-energy electron scattering and transport in metals

B. Solleder\textsuperscript{1}, C. Lemell\textsuperscript{1}, K. Tókési\textsuperscript{2}, N. Hatcher\textsuperscript{3} and J. Burgdörfer\textsuperscript{1}

\textsuperscript{1} Institute for Theoretical Physics, Vienna University of Technology, 1040 Vienna, Austria, EU
\textsuperscript{2} Institute of Nuclear Research of the Hungarian Academy of Sciences, (ATOMKI), H–4001 Debrecen, P.O.Box 51, Hungary, EU
\textsuperscript{3} Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60208-3112, USA

E-mail: beate@concord.itp.tuwien.ac.at

Abstract. We study spin-dependent scattering and transport of low energy electrons ($\leq 500$ eV) through metals employing a classical transport theory within which electron trajectories are simulated as a sequence of stochastic scattering events. Elastic as well as spin-dependent inelastic processes are included in our model simulating the complete secondary electron cascade. We apply our model to spin-polarization measurements of electrons emitted from magnetized Fe after impact of unpolarized primary electrons. We find good agreement with experimental data.

1. Introduction

Probing magnetized materials is, apart from conceptual aspects, important in view of numerous technical applications ranging from spintronics to optimized data storage devices. In the last decades, different experimental techniques have been developed to study the properties of magnetized materials such as photoemission [1] or electron spectroscopy [2]. Surface effects are investigated using electron or ion scattering under grazing incidence conditions, where the polarization of emitted radiation [3] or the spin polarization of emitted electrons [2, 4, 5] comprise information about the material properties.

A complete theoretical description of the underlying physical processes is a challenging task in view of the large number of particles and degrees of freedom involved. Several attempts have been made reaching qualitative agreement with the experiment (e.g. [6, 7, 8]), however, relying on free parameters adjusted to experimental results. In our work we attempt a full microscopic description of electron scattering and transport in magnetized materials, taking magnetized iron as an example, where we focus on electron energies below 500 eV.

Our work was motivated by a secondary electron emission experiment by Kirschner et al. [2], where the spin polarization of emitted low-energy electrons was measured after impact of an unpolarized electron beam on a magnetized iron surface. They found a strong positive polarization of electrons for emission energies below 30 eV, which originates, as we will show in this work, from the spin polarization of both the occupied and the unoccupied band structure, where the latter is responsible for an inelastic spin-filter process active in the few-eV range.

Our study of spin-dependent electron transport is also motivated by experimental data for the interaction of highly charged ions (HCI) with magnetized surfaces [5, 9]. There, the low-energy
electron emission spectrum is composed of directly emitted electrons produced by potential and kinetic emission as well as of secondary electrons excited below the surface. In collisions of HCI with magnetized iron the polarization of emitted electrons was found to be even higher than in electron spectroscopy. The present study is the first step towards a full spin-dependent description of ion-surface collisions.

In this special report we present first numerical results of our electron transport simulation and a comparison with experimental data of Kirschner et al. Atomic units (a.u.) are used unless stated otherwise.

2. Theoretical model

Electrons impinging on a solid are either elastically backscattered at the surface or penetrate into the bulk. There they undergo a sequence of elastic and inelastic scattering events before they are either reemitted or stopped in the bulk. The electrons are elastically scattered at the screened core potentials of the lattice ions, \( V(r) \), approximated by a muffin-tin model potential (Fig. 1 a). While in an elastic process only momentum is transferred, energy is exchanged between the projectile electrons and the electronic system of the solid in an inelastic collision (Fig. 1 b). Additional excitation channels open near the surface due to the breaking of symmetry at the solid-vacuum interface. These surface excitations dominate the inelastic processes in the vicinity of the surface, while bulk excitations dominate at distances a few a.u. below. Secondary electrons are created, when the amount of transferred energy is large enough for the excitation of a target electron into an unbound state.

Following the classical transport theory (CTT [10]) for open systems, the electronic dynamics is represented by a classical phase-space distribution \( f(\mathbf{r}, \dot{\mathbf{r}}, t) \). Its time evolution is determined by the corresponding Langevin equation

\[
\ddot{\mathbf{r}}_i = -\nabla V(\mathbf{r}_i, t) + \mathbf{F}_{stoc}(\mathbf{r}_i, \dot{\mathbf{r}}_i, t),
\]

which we solve for representative trajectories \( i = 1, ..., N_E \) employing classical trajectory Monte Carlo (CTMC) simulations. Here, \( N_E \) is the number of particles in the ensemble. \( \mathbf{F}_{stoc} \) are...
stochastic forces representing the collisions, which are treated as Poissonian stochastic processes. The stochastic forces are derived from the collision kernels of the associated Liouville-Master equation, determined either from ab initio quantum calculations or independent experimental data. Conservative forces, indicated in Eq. 1 by $-\vec{\nabla}V(\vec{r}_i)$, e.g. the crystal field, are neglected in the present work but could be included straightforwardly, if needed. $F_{\text{stoc}}$ is expressed in terms of impulsive momentum transfers at discrete times of different collision processes. Which type of collision happens is determined by the inverse mean free path ($\lambda_I^{-1}$), where $\alpha$ represents elastic, inelastic bulk, or inelastic surface excitations. Elastic collisions are the dominant channel showing the smallest MFP ($\lambda_e$) for most energies (Fig. 2). The inelastic MFPs depend on the distance $z$ to the surface, where the inverse surface MFP, $\lambda_s^{-1}$, decreases towards the bulk, while inelastic bulk excitations become less important towards the surface. Fig. 2 shows the minimum values of these MFPs, i.e. $\lambda_s$ at the surface and the bulk inelastic MFP $\lambda_{in}$ in the bulk.

In our simulation we follow the trajectories of the primary projectiles as well as secondary electrons and electrons of further generations, i.e. the entire collision cascade. The number of particles in the ensemble, $N_E$, is therefore not conserved but increases during the collision cascade. We follow two subensembles of opposite spin, where we allow electrons to be exchanged between the subensembles of spin-up and spin-down electrons due to inelastic spin-flip processes described below.

For the material and the energy range considered in our work, the spin dependence of elastic scattering can be neglected [11]. Spin effects are restricted to inelastic processes. They originate from the spin density of states (SDOS) of the target conduction band. Magnetized materials show an energy shift $\Delta$ (exchange splitting) between spin-up and spin-down states (Fig. 3 [11]). As a consequence, more majority than minority states are occupied by conduction band electrons leading to a positive mean polarization $\bar{P}$ averaged over the conduction band, which in the case of iron is $\bar{P} \approx 35\%$. The polarization $P$ is defined as $P = (N_{\uparrow} - N_{\downarrow}) / (N_{\uparrow} + N_{\downarrow})$, where $N_{\uparrow(\downarrow)}$ is the number of spin-up (down) electrons. Here, spin up (majority) means parallel and spin down (minority) means antiparallel to the direction of magnetization. The occupied part of the SDOS constitutes, up to a normalization factor, the energy and spin distributions of excited secondary electrons, where the bulk SDOS is used for bulk excitations while the SDOS of the topmost atomic layer is used in the case of surface excitations (Fig. 3). As secondary electrons reflect, on average, the spin polarization of the conduction band, a positive polarization is also expected for the few-eV range of the emission spectrum where secondaries dominate. For very low energies, the polarization is additionally enhanced by so-called Stoner excitations originating from the excess of unoccupied minority spin states in the conduction band (Fig. 3). With decreasing

![Figure 2](image-url)
primary energy these unoccupied states become increasingly important as final states in inelastic scattering. As minority electrons find a much larger number of final states, scattering of spin-down electrons is preferred. On the other hand, the probability for exciting secondary electrons of majority spin is enhanced, so that Stoner excitations appear as an effective spin-flip inelastic process. This leads to a shorter inelastic MFP for minority electrons which causes a spin-filter effect at very low energies. To determine the spin dependence of $\lambda_{in}$ we distinguish between final states above and below the vacuum level $E_v$, where only the latter case leads to a spin dependence of $\lambda_{in}$ due to the spin asymmetry in the unoccupied states of the conduction band. Final states above $E_v = E_F + W$ are equally accessible for both spin-up and spin-down electrons ($W$ is the work function of the solid). Accordingly, the inverse inelastic MFP can be expressed as a sum of a spin-independent contribution $\lambda_{> E_v}^{-1}$ corresponding to final states above $E_v$ and a spin-dependent contribution $\lambda_{< E_v, \uparrow(\downarrow)}^{-1}$ representing inelastic scattering to final states in the polarized conduction band [11],

$$\lambda_{in, \uparrow(\downarrow)}^{-1} = \lambda_{> E_v}^{-1} + \lambda_{< E_v, \uparrow(\downarrow)}^{-1},$$

(see Fig. 2). The spin dependence of $\lambda_{< E_v, \uparrow(\downarrow)}$ is determined by the spin asymmetry in the unoccupied part of the SDOS.

Stoner excitations are only included in bulk excitations. Their inclusion in surface excitations would require a detailed knowledge of the SDOS as a function of the distance to the surface, which is currently not yet available. We plan to include spin dependent surface excitations in the near future.

### 3. Application to Fe

As a first test of our model, we compare our results for the absolute electron yield resulting from electron scattering at an iron surface with the measured data of Kirschner et al. [2]. Both the calculated and measured total secondary electron yield (Fig. 4) increase with primary electron energy towards a maximum at about 500 - 600 eV. Although a further increase of the primary energy increases the number of secondary electrons in the bulk, the observed electron yield does not increase further. As a result of the larger penetration depth of the primary electron, more secondaries are produced too far inside the solid as to reach the surface during transport. The energy dependence of the simulated yield closely follows the experimental data while exceeding the yield by about 30% which may be a consequence of the limited collection efficiency in the

---

**Figure 3.** (Color online) Spin density of states (SDOS) for a) paramagnetic, b) ferromagnetic bulk and c) ferromagnetic surface Fe. The magnetic SDOS is characterized by an energy shift $\Delta$ (exchange splitting) between minority and majority states. The unoccupied states between $E_F$ and the $E_F + W$ are spin dependent final states in inelastic scattering.
For the comparison of our polarization data with the experiment, we focus on the results for primary energies $E_p$ below 500 eV. Fig. 5 a shows the average spin polarization of emitted electrons after impact of unpolarized primary electrons with $E_p = 90$ eV and $E_p = 500$ eV. Two significant features are observed in the experiment and reproduced in our simulations: increasing polarization with increasing primary energy, and increasing polarization with decreasing emission energy. The former is a consequence of the composition of the emission spectrum, which is dominated by secondary electrons in this energy range but still contains contributions from backscattered primary electrons. These primaries keep their polarization $P_p = 0$ to a large extent while secondaries are emitted with the average conduction band ($P_s$) or even higher polarization, if they have undergone Stoner excitations, $P_s \geq P_s \approx 35\%$. Backscattered primaries in the low energy emission spectrum therefore reduce the polarization. The lower the primary energy, the more backscattered primaries still end up in the emission spectrum causing lower degrees of polarization. If the fraction of backscattered primaries becomes negligible, the polarization saturates, which is not yet the case at $E_p = 500$ eV [11] but was experimentally found to be at about $E_p = 1$ keV [2]. To illustrate the role of Stoner excitations, results of calculations neglecting this effect are also depicted in Fig. 5 a. Due to Stoner excitations low-energy spin down electrons are filtered out during transport as they have a shorter MFP. This spin-filter effect leads to an additional steep increase of the polarization in the few-eV range.

A discrepancy between the experiment and the simulation in the shape of the polarization data is found between 10 and 20 eV, where a systematically higher polarization was measured. In the experiment, it was ruled out that this feature originates from surface effects [2]. Crystalline effects are also unlikely to be the origin since the polarization data have been found to be insensitive to the emission angle. As the energy window coincides with the electron energy expected for plasmon decay into particle-hole excitations ($\omega_p \approx 15$ eV), it is suggestive to relate this feature to the decay of volume plasmons. A plausible hypothesis for plasmon decay is that electron-hole excitations occur preferentially near the Fermi edge, which minimizes the momentum transfer required for the decay to take place. As the polarization at the Fermi edge ($P_{E_F} \approx 40\%$) is higher than the mean conduction band polarization, this selective decay would enhance the polarization in the considered emission energy window. We have tested our hypothesis by slightly increasing the probability to excite secondaries around the Fermi edge [11], if $\omega$ approximately coincides with the plasmon frequency, leading to the results shown in Fig. 5 b. The improved agreement with experiments favors our hypothesis. However, a detailed treatment of this phenomenon is to our knowledge still missing but required to validate this hypothesis.
Figure 5. (Color online) a) Spin polarization of emitted electrons from a magnetized Fe surface bombarded with 90 eV and 500 eV unpolarized electrons. ○ experimental results [2]; • present simulation. – – – polarization results neglecting Stoner excitations. b) Same as a) including the additional polarization contribution due to plasmon decay near the Fermi edge (see text).

Acknowledgments
This work was supported by the Austrian Fonds zur Förderung der wissenschaftlichen Forschung (FWF Austria) under project no. P17449-N02, by EU under contract no. HPRI-CT-2005-026015, the Hungarian Scientific Research Fund: OTKA nos. T046095, T046454, the grant “Bolyai” from the Hungarian Academy of Sciences, the Hungarian National Office for Research and Technology, and the Stiftung Aktion Österreich-Ungarn no. 67013.

References

[1] Long R L, Jr., Hughes V W, Greenberg J S, Ames I and Christensen R L 1965 Phys. Rev. 138 A1630
[2] Kirschner J and Koike K 1992 Surf. Sci. 273 147
[3] Unipan M, Winters D F A, Robin A, Morgenstern R and Hoekstra R 2005 Nucl. Instr. Meth. Phys. Res. B 230 356
[4] Lancaster J C, Kontur F J, Walters G K and Dunning F B 2003 Phys. Rev. B 67 115413
[5] Pfandzelter R, Bernhard T and Winter H, 2001 Phys. Rev. Lett. 86 4152
[6] Penn D R, Apell S P and Girvin S M 1985 Phys. Rev. Lett. 55 518
[7] Yasuda M, Tamura K, Kawata H and Murata K 2001 J. Phys. D: Appl. Phys. 34 1955
[8] Sun X and Ding Z 2005 J. Phys. D: Appl. Phys. 38 456
[9] Solleder B, Lemell C, Tókési K and Burgdörfer J 2007 Nucl. Instr. Meth. Phys. Res. B 258 130
[10] Burgdörfer J and Gibbons J 1990 Phys. Rev. A 42 1206, Deiss C et al. 2006 Phys. Rev. Lett. 96 013203
[11] Solleder B, Lemell C, Tókési K, Hatcher N and Burgdörfer J 2007 accepted for Phys. Rev. B
[12] Weinert M, Wimmer E and Freeman A J 1982 Phys. Rev. B 26 4571, Jansen H J F and Freeman A J 1984 Phys. Rev. B 30 561
[13] Perdew J P, Burke K and Ernzerhof M 1996 Phys. Rev. Lett. 77 3865
[14] Salvat F, Jablońska A and Powell C 2005 Comp. Phys. Comm. 165 157
[15] Reinhold C O and Burgdörfer J 1997 Phys. Rev. A 55 450
[16] Ding Z J and Shimizu R 1989 Surf. Sci. 222 313
[17] Lynch D W and Hunter W R 1991 Handbook of Optical Constants of Solids vol 2 ed E D Palik (Academic Press) pp385-396
[18] Ritchie R H and Marusak A L 1966 Surf. Sci. 4 234