Influence of spin–orbit coupling on the momentum distribution of electron pairs emitted from Au on Ir(111)

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Abstract

We explore by theory and experiment the effects of spin–orbit coupling (SOC) on the pair creation of electrons by spin-polarized primary electrons incident on a pseudomorphic monolayer of Au on Ir(111). An ab-initio calculation of the electronic structure reveals a Rashba-type sp-like surface state in the Au layer, which turns out to lead to a large electron pair creation intensity. The distribution of this intensity over the momenta of the emitted electrons depends strongly on the primary electron spin due to spin–orbit coupling mainly in the incident and the outgoing electron states. For normal incidence, the six-fold rotation symmetry, which would hold without spin–orbit coupling, is broken in a manner depending on the orientation of the primary electron spin.

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1. Introduction

The spin-dependence of electron-electron scattering in solids is generally brought about by spin–orbit and exchange interaction in the one-electron states as described by a Dirac equation with an effective magnetic field. For experimental studies two limiting cases are most useful: (a) scattering of polarized electrons from low-Z ferromagnets, which emphasizes the exchange interaction and (b) scattering of polarized electrons from high-Z non-magnetic solids, which singles out the spin–orbit interaction. The former case was harnessed a few years ago for a study of the exchange-correlation hole in the near-surface region of Fe(100) [1]. In the present paper we study the spin dependence of the electron pair intensity distribution due to electron scattering from a pseudomorphic monolayer of Au grown on Ir(111).

The basic idea is to send an electron of at a well-defined angle, energy and spin state on to a single-crystal surface of a sufficiently high-Z material in order to observe effects of spin–orbit coupling (SOC) in the scattering process. If the primary energy is high enough relative to the binding energy of a valence electron we may detect two electrons emitted from the surface. Hence the terminology (e,2e). We call the two electrons “a pair” because they are correlated with respect to their momenta, their total energy and their spin. The pair creation is experimentally studied by detecting the two electrons in coincidence on two detectors within a time window of a few nanoseconds. The spin dependence of this pair creation process is obtained by a second measurement where the primary electron spin is reversed. The resulting normalized difference of the pair creation rates gives rise to a “spin asymmetry”. For comparison with experiment and for further analysis, spin-dependent (e,2e) rates were calculated by means of a relativistic multiple scattering formalism.

Experimental and theoretical (e,2e) results for Au on Ir(111) are presented in the form of distributions of the spin-averaged pair creation rate (“intensity”) and of the difference between spin-up and spin-down rates (“intensity difference”) over the momenta of the two emitted electrons (“momentum distributions”). In particular, we ask the following questions. (1) Can SOC substantially alter the symmetry of the momentum distributions? The answer is “yes” (see Section 5). (2) Can SOC significantly affect the extension of the exchange-correlation hole? The answer is “yes” or “no” depending on the primary electron energy (see Section 5).

2. Experiment

The experimental setup is shown schematically in Fig. 1. It consists of two channelplates and a spinpolarized electron source [2]. The photocathode is excited by light pulses from a diode laser [3] (pulse width of a few tenths of a nanosecond, repetition rate up to 20 MHz). At the exit of the gun we obtain a flux of single electrons which are sent to the target. The energy spectrum of the scattered...
electrons is determined by the time difference between the trigger to the light source and the electronic pulse from the anode of each of the channelplates. If the primary electron creates an electron pair the faster one opens a time window and the slower one closes it. If this happens we detect a coincidence event for a pair of electrons within this time window. We thus have a start pulse from the laser pulse trigger and two stop pulses. From this we calculate the electrons’ flight times and from that the electrons’ energies. The electronic signals are digitized by a fast digitizer [4] and analyzed by a PC running LabView software.

Each of the channelplates is equipped with a double delay line [5]. The delay line signals are also digitized, triggered by the ‘coincidence event’ signal. From the delay line signals (difference and sum) we compute the location of each electron impact on the channelplate. These spatial informations are used (a) for a correction of the flight paths (shorter for an impact near the center of the anode and longer near its edge) and (b) for the determination of the angle at which an electron leaves the target surface. From this we determine the momentum of each electron within a pair. Overall we obtain a spatio-temporal resolution of typically 0.5 mm and 0.5 ns respectively for each coincidence event. The typical coincidence pair event rate is between one and ten per second.

As a sample we decided to use the pseudomorphic monolayer of Au on Ir because of some special properties: this system grows layer-by-layer, as first observed by Thomas in 1972 [6] and it is easy to produce a monolayer of Au on the surface. One first deposits a multilayer of Au on Ir by evaporation. The binding energy of Au on Au is lower than that of Au on Ir. Expressed in desorption temperature the Au desorption from Au occurs at 100°C to 200°C less than the desorption of Au from Ir (880°C versus 880°C). Therefore we apply a series of flashes at 860°C until only a monolayer of Au remains [7]. The LEED pattern then is p(1 x 1) [8]. In the 10–100 mbar vacuum range this surface stays clean for more than 15 months. The adsorbed Au can be completely removed at about 1200°C. A pseudomorphic Au monolayer is restored reliably by repeating the above procedure. A drawback of the high temperature flashes is that the crystal holder tends to creep slightly. After many cycles this creep came to rest at a crystal tilt angle of 4° (see below).

3. Theoretical methods

For the computation of spin-dependent (e,2e) momentum distributions from Au on Ir(001) we employed a formalism, which has been presented in detail in earlier work (c.f. [9,10]). We therefore only briefly recall its key features and formulae.

A primary electron with energy \( E_1 \), surface-parallel momentum component \( \vec{k}_1^s \) and spin orientation \( \sigma_1 \) relative to an axis \( \vec{e} \) (i.e. spin polarization vector \( \vec{P}_1 = \sigma_1 \vec{e} \) at the electron gun) collides with a valence electron with energy \( E_2 \), surface-parallel momentum component \( \vec{k}_2^s \) and spin label \( \sigma_2 \), and two outgoing electrons with \( (E_2, \vec{k}_2^s, \sigma_3) \) and \( (E_4, \vec{k}_4^s, \sigma_4) \) are detected. The four one-electron states \( (E_i, \vec{k}_i^s, \sigma_i) \), in the following written as \( |i\rangle \), with \( i=1,2,3,4 \) are solutions of the Dirac equation with a complex effective potential. The primary electron state \( |1\rangle \) is a low-energy electron diffraction (LEED) state and the outgoing electron states \( |3,4\rangle \) are time-reversed LEED states. While these states have definite spin orientation \( \sigma_i \) at the source and at the two detectors, respectively, inside the solid they involve parts with \( \sigma_i \) and parts with \( -\sigma_i \) as a consequence of spin–orbit coupling. For the valence electron state \( |2\rangle \), \( \sigma_2 \pm \) is in general only a label to characterize two degenerate states involving spin–orbit coupling. The initial two-particle state \( |1,2\rangle \) is an antisymmetrized product of states \( |1\rangle \) and \( |2\rangle \). The final two-electron state \( |3,4\rangle \) includes the Coulomb correlation between the one-electron states \( |3\rangle \) and \( |4\rangle \) (as described in detail in [10]).

For a spin-polarized primary beam impinging on a surface system, the spin-dependent \( (e,2e) \) scattering cross section (“intensity”) is then given by the golden rule form

\[
I^{(1)}(E_1, \vec{k}_1^s, E_2, \vec{k}_2^s, E_4, \vec{k}_4^s) = \frac{k_1 k_2}{\epsilon_1 \epsilon_2 \epsilon_3} \sum_{n_1,n_2} \left| \langle 3,4|U|1,2 \rangle \right|^2 \delta, \tag{1}
\]

where \( k_i = \sqrt{2E_i} \) for \( i=1,3,4 \) and \( U \) is the screened Coulomb interaction. In the summation over the valence states \( |2\rangle \) the index \( n_2 \) accounts for possible further degeneracies. \( \delta \) symbolizes the conservation of energy and surface-parallel momentum

\[
E_1 + E_2 = E_3 + E_4 \quad \text{and} \quad \vec{k}_1^s + \vec{k}_2^s = \vec{k}_3^s + \vec{k}_4^s + \vec{g}, \tag{2}
\]

where \( \vec{g} \) is a surface reciprocal lattice vector. For fixed energies and parallel momenta of the primary electron and of the two detected electrons, one thus “picks out” valence electrons with definite energy and parallel momentum.

To perform numerical \((e,2e)\) calculations for a specific surface system, the geometrical and the electronic structure of the ground state are required. To obtain these, we employed an ab-initio full-potential linear augmented-plane-wave (FLAPW) method [11], using a local density approximation (LDA) for the exchange-correlation energy [12]. Geometry and electronic densities of states results for Au/Ir(111) will be presented in Section 4. Further, the ab-initio calculation provided a real one-electron potential, which we used to construct the complex quasi-particle potential input for our \((e,2e)\) calculations.

4. Geometrical and electronic structure

As described in Section 2, our surface system is a pseudomorphic monolayer of Au on Ir(111). The Au layer thus has the same surface-parallel unit cell as the Ir layers and the Au atoms are all within a single plane. To determine the spacing between the Au layer and the topmost Ir layer and the spacings between the near-surface Ir layers we resorted to an ab-initio calculation by the full-potential linearized augmented plane wave method with a local density approximation for the exchange-correlation energy [12] as implemented in the Juelpich FLEUR computer code [11]. For a 31-layer film, which consists of 29 Ir layers and an Au monolayer on each side, we allowed the three topmost interlayer spacings to relax such that the total energy became minimal and the forces on the atoms were practically zero.

For the spacing between the Au layer and the topmost Ir layer we thus obtained 2.41 Å, which is larger than the interlayer spacing in bulk Ir (2.22 Å), and also larger than the interlayer spacing in bulk Au (2.36 Å) due to the lateral compression of the Au layer. The spacing between the first and second Ir layer is 2.15 Å and that between the second and third Ir layer is 2.19 Å, i.e. both are somewhat less than the bulk Ir spacing 2.22 Å.
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