Orientation-Dependent Transparency of Metallic Interfaces

P. X. Xu,[1] K. Xia,[1] M. Zwierzycki,[2,3,*] M. Talanana,[2] and P. J. Kelly[2]

[1]*State Key Laboratory for Surface Physics, Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100080, China*

[2]*Faculty of Science and Technology and MESA$^+$ Institute for Nanotechnology, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands*

[3]*Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*

(Received 12 December 2005; published 2 May 2006)

As devices are reduced in size, interfaces start to dominate electrical transport, making it essential to be able to describe reliably how they transmit and reflect electrons. For a number of nearly perfectly lattice-matched materials, we calculate from first principles the dependence of the interface transparency on the crystal orientation. Quite remarkably, the largest anisotropy is predicted for interfaces between the prototype free-electron materials silver and aluminum, for which a massive factor of 2 difference between (111) and (001) interfaces is found.

DOI: 10.1103/PhysRevLett.96.176602 PACS numbers: 72.10.Bg, 71.15.−m, 72.25.Ba, 73.40.−c

A recurring theme in condensed matter physics in the past 20 years has been the discovery of new physical effects and properties in systems with reduced dimensions; the prospect of exploiting these effects and properties in logical processing, sensing, and storage devices is an important driving force behind nanoscience and nanotechnology. In semiconductors, the electronic structures of the electrons responsible for conduction can be described using simple models. The same is not true of the ferromagnetic transition metals, which form the basis for magnetoelectronics. It is the nontrivial spin dependence of the transmission and reflection of electrons at magnetic interfaces which provides the key to understanding phenomena such as oscillatory exchange coupling, giant and tunneling magnetoresistance, spin transfer torque, spin pumping, and spin injection [1]. For well-studied material combinations such as Co/Cu and Fe/Cr, modest spin dependence of the interface transmission [2–4] of the order of 10%–20% is sufficient to account for experimental observations [5].

However, the confrontation of theory and experiment just referred to is at best indirect and model-dependent. Even though the theory of transport in small structures is formulated in terms of transmission and reflection matrices [6], measuring interface transparencies directly has proven quite difficult [7]. To identify interfaces suitable for experimental study, we have undertaken a systematic materials-specific study of the orientation dependence of the interface transmission between pairs of isostructural metals whose lattice constants match within a percent or so in the hope that it will prove possible to grow such interfaces epitaxially.

One of the metal pairs we studied was Al/Ag. Both metals have the fcc crystal structure, and their lattice constants are matched within 1%. Aluminum is a textbook [8] example of a system well described by the (nearly) free-electron model. Silver, also usually assumed to be a free-electron-like material, is a noble metal with high conductivity which is frequently used for electrical contacting. We found that, in spite of the simplicity of both metals' electronic structures, the transmission through Al/Ag interfaces can differ quite significantly from the predictions of the free-electron model. In particular, between (111) and (001) orientations, we find a factor of 2 difference in interface transmission for clean Al/Ag interfaces. For free electrons, the anisotropy should vanish. Our result is insensitive to interface disorder. We identify a new factor responsible for this difference which is not related to the standard velocity- [9,10] or symmetry-mismatch [11,12] mechanisms.

A free-electron description of interface scattering, in which the effect of the crystal potential on transport is completely neglected, underlies the Blonder-Tinkham-Klapwijk theory [13] used to interpret [9,10] Andreev reflection (AR) experiments. Point contact AR experiments are increasingly used to identify the pairing symmetry of superconductors and, in the field of magnetoelectronics, to determine the polarization of magnetic materials [14,15]. Our finding that the electronic structure can have such a large effect on the interface transmission implies that experiments should be analyzed using more sophisticated models.

Our study was based upon first-principles calculations of the interface electronic structure performed within the framework of density functional theory and the local spin density approximation. Bulk and interface potentials were determined self-consistently using the tight binding linearized muffin tin orbital (TB-LMTO) [16] surface Green's function method [17]. We assumed common lattice constants for both metals of a given structure; e.g., $a_{\mathrm{Al}} = a_{\mathrm{Ag}} = 4.05$ Å. The potentials obtained in this way were used as input to a TB-MTO wave-function-matching [4,12] calculation of the transmission and reflection coefficients between Bloch states on either side of the interface. The efficiency of this approach is such that interface disorder can be modeled using large lateral supercells. For disordered systems, the potentials were calculated using the layer coherent potential approximation. The results of the

calculations for a number of lattice-matched materials are summarized in Table I.

The Sharvin conductances G_A and G_B, reported in the third and fourth columns in Table I, are proportional to the number of states at the Fermi level propagating in the transport direction. They are properties of the bulk materials which are determined by the area of the Fermi surface projections and are a measure of the current-carrying capacity of the conductor in the ballistic regime. The largest intrinsic orientation dependence, seen to be about 13%, is found for W; for Al and Ag, respectively, it is less than 8% and 5%.

The interface transmission in column five in Table I is expressed as a conductance $G_{A/B} = e^2/h\sum_{\mu\nu} T_{\mu\nu}$, where $T_{\mu\nu}$ is the probability for the incoming state ν in material A to be transmitted through the interface into the outgoing state μ in material B. For most pairs of materials [18], the orientation dependence of $G_{A/B}$ is modest ($\sim$15% for Mo/W) and the interface conductance itself tends to be slightly smaller than the lower of the two Sharvin conductances. For these systems, the behavior of the transmission appears to be determined by the projection of the Fermi surfaces. However, this is not so for Al/Ag and Al/Au interfaces. Here we observe a large anisotropy in the transport properties. The factor of 2 difference in transmission between (111) and (001) orientations [19] results in a factor of 4 difference between interface resistances estimated using the method of Refs. [2,4].

The transmission probability for the (111) and (001) orientations is plotted in Figs. 1(c) and 1(f) as a function of the wave-vector component parallel to the interface $\mathbf{k}_\parallel$, within the 2D interface Brillouin zones (BZ). A qualitative difference between the two orientations can be observed. In the (111) case, the transmission is almost uniformly high wherever there are states on both sides of the interface. The (001) orientation exhibits more variation with high transmission in the central and outer regions of the 2D BZ but much lower in a ring-shaped region in between. The presence of this ''cold ring'' is the reason the total transmission is lower for the (001) orientation. Explaining the transparency anisotropy of Al/Ag interfaces requires finding an explanation for the low transmission values in this region of the 2D BZ.

Two mechanisms are usually taken into account when analyzing the scattering at perfect interfaces. The first, velocity mismatch, is the modulation of the transmission by a factor reminiscent of the free-electron formula for the transmission through a potential step: $T = 4v_L v_R/(v_L + v_R)^2$,

TABLE I. Sharvin conductances and interface transmissions in units of $10^{15}\ \Omega^{-1}\,\mathrm{m}^{-2}$; interface resistances SR [2,4] for ideal (ordered) interfaces in units of $10^{-15}\ \Omega\,\mathrm{m}^2$. S is the area of the sample for which R is measured. Interface disorder was modeled in 10×10 lateral supercells with two layers of a 50-50 alloy. The largest uncertainty between different configurations of disorder is about 2.3%. The values given are for a single spin. For the pairs of materials and orientations indicated by a (*), comparison of the interface resistances shown in the last two columns with experimental values extracted from measurement on multilayers by the Michigan State University group [5,7] yields reasonable quantitative agreement [2,4,12].

A/B		G_A	G_B	$G_{A/B}$	$2SR$
Al/Ag	(111)	0.69	0.45	0.41 (0.36)	0.64 (0.92)
$a_{\mathrm{fcc}} = 4.05$ Å	(110)	0.68	0.47	0.30 (0.32)	1.60 (1.39)
	(001)	0.73	0.45	0.22 (0.24)	2.82 (2.37)
Al/Au	(111)	0.69	0.44	0.41 (0.35)	0.60 (0.99)
$a_{\mathrm{fcc}} = 4.05$ Å	(001)	0.73	0.46	0.24 (0.26)	2.37 (2.14)
Pd/Pt	(111)	0.62	0.71	0.55 (0.54)	0.30 (0.33)
$a_{\mathrm{fcc}} = 3.89$ Å	(001)	0.58	0.70	0.52 (0.51)	0.37 (0.39)
W/Mo	(001)	0.45	0.59	0.42 (0.42)	0.42 (0.42)
$a_{\mathrm{bcc}} = 3.16$ Å	(110)	0.40	0.54	0.37 (0.38)	0.52 (0.47)
Cu/Co	(111)*	0.56	0.47	0.43 (0.43)	0.34 (0.35)
Majority	(001)	0.55	0.49	0.46 (0.45)	0.26 (0.27)
$a_{\mathrm{fcc}} = 3.61$ Å	(110)	0.59	0.50	0.46 (0.46)	0.35 (0.35)
Cu/Co	(111)*	0.56	1.05	0.36 (0.31)	1.38 (1.82)
Minority	(001)	0.55	1.11	0.32 (0.32)	1.79 (1.79)
$a_{\mathrm{fcc}} = 3.61$ Å	(110)	0.59	1.04	0.31 (0.35)	1.89 (1.55)
Cr/Fe	(111)	0.61	0.82	0.27 (0.31)	2.22 (1.84)
Majority	(001)	0.64	0.82	0.11 (0.25)	7.46 (2.55)
$a_{\mathrm{bcc}} = 2.87$ Å	(110)*	0.59	0.78	0.22 (0.27)	3.04 (2.18)
Cr/Fe	(111)	0.61	0.41	0.34 (0.34)	0.93 (0.95)
Minority	(001)	0.64	0.46	0.35 (0.35)	0.98 (0.95)
$a_{\mathrm{bcc}} = 2.87$ Å	(110)*	0.59	0.40	0.32 (0.32)	1.03 (1.06)

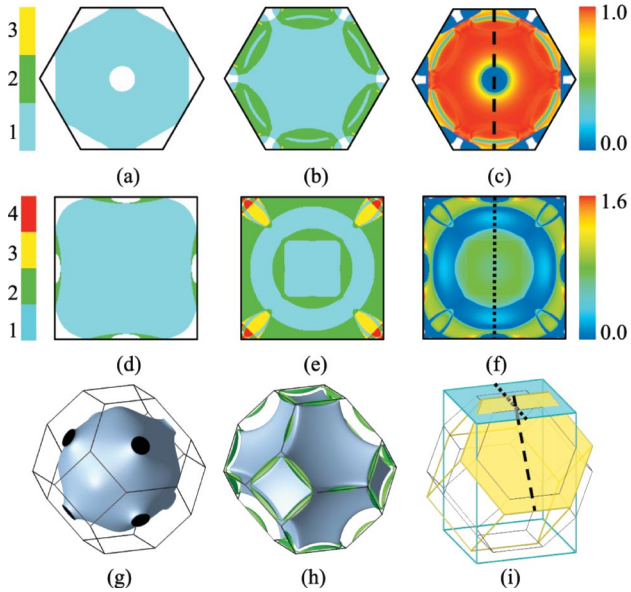

FIG. 1 (color). Top row: Fermi surface projections for (a) Ag, (b) Al, and (c) transmission probabilities in the 2D BZ for the (111) orientation. Middle row: Same for the (001) orientation. The color bars on the left indicate the number of scattering states in the leads for a given two-dimensional wave vector $\mathbf{k}_\parallel$. The transmission probabilities indicated by the color bars on the right can exceed 1 for $\mathbf{k}_\parallel$s for which there is more than one scattering state in both Ag and Al. Bottom row: Fermi surfaces of (g) Ag and (h) Al, (i) the interface-adapted BZ for (001) and (111) orientations. The vertical dashed line in (c) and on the yellow plane in panel (i) indicate the cross section used in the left-hand panel in Fig. 2, while the vertical dotted line in (f) and on the blue plane in panel (i) indicate the cross section used in the right-hand panel.

where $v_{L/R}$ are the components of the Fermi velocities in the transport direction on the left and right sides of the interface. This modulation is indeed present in our calculated transmissions, but its effect tends to be noticeable only when one of the velocities is almost vanishingly small. Naive application of the free-electron formula yields uniformly good transmission [20] independent of the orientation. Symmetry mismatch, the second mechanism, can suppress the transmission between states of incompatible symmetries (e.g., even vs odd, etc.). Examination of the eigenvectors demonstrates that this is not the case for the Al/Ag system. For example, states on both sides of the interface, with $\mathbf{k}_\parallel$ along the vertical dotted line in Fig. 1(f), are even under reflection in the plane defined by this line and the (001) transport direction. Their orbital composition (s, p_y, p_z, d_{yz}, $d_{3z^2-r^2}$, $d_{x^2-y^2}$, where the y axis is parallel to the dotted line and z is the transport direction) is essentially the same for both materials. The same holds for states along other symmetry lines or planes and general $\mathbf{k}_\parallel$ points (in the sense of orbital composition). The origin of the cold ring must be sought elsewhere.

In spite of the failure of the free-electron transmission formula, this simple model serves as a useful starting point for analyzing the Fermi surface (FS) topologies. In the simplest possible approach, we model the FS of Ag [shown in Fig. 1(g)] as a sphere which fits into the first BZ. A larger sphere, accommodating three electrons, is needed for trivalent Al. In an extended zone scheme, conservation of momentum parallel to the interface dictates that the transmission through a specular interface is nonzero only between states with the same values of $\mathbf{k}_\parallel$; these are the $\mathbf{k}_\parallel$ vectors belonging to the region where projections of the Fermi spheres on a plane perpendicular to the transport direction overlap. For systems with lattice periodicity, we must use a downfolded FS, with fragments of the original FS sphere backtranslated into the 1st Brillouin zone, a procedure which can be realized geometrically by placing spheres accommodating three electrons on reciprocal lattice (RL) sites and then only considering the fragments in the first BZ. Examination of the FS of Al calculated from first principles [Fig. 1(h)] and its cross section (Fig. 2) reveals that, in spite of its apparent complexity, it remains essentially (piecewise) spherical. For some values of $\mathbf{k}_\parallel$ [see Figs. 1(b) and 1(e)], Al can now have more than one propagating state. Nevertheless, in the free-electron limit, the downfolded states are strictly orthogonal to the states in Ag and the total transmission is unchanged. For a reduced zone scheme, we formulate the following rule: The transmission between states in two (nearly) free-electron materials which have the same $\mathbf{k}_\parallel$ but originate from reciprocal lattice sites whose parallel components do not coincide vanishes in the free-electron limit and is expected to be strongly suppressed for nearly free-electron-like materials.

Obviously, the truly free-electron system cannot exhibit anisotropy. However, in the presence of the periodic potential, the original, piecewise-spherical Fermi surface and, consequently, the transmission are going to be modified. First, since the wave functions are no longer pure plane waves, the strict orthogonality of the downfolded states is relaxed and the transmission can assume finite although

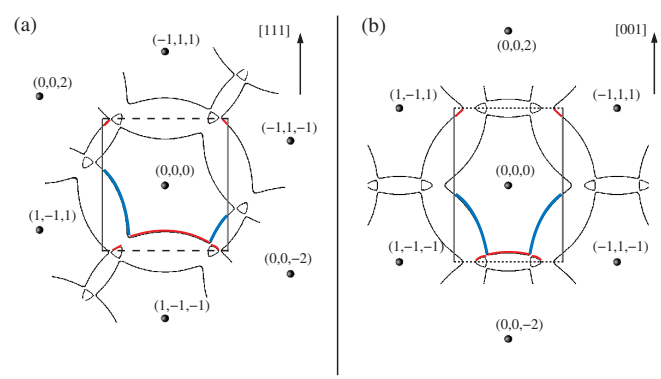

FIG. 2 (color). Intersection of a (110) plane with the Al Fermi surface and with the interface-adapted BZs indicated in Fig. 1(i) (where the meaning of the dashed and dotted lines is explained). The labeled dots indicate the positions of the RL sites with coordinates given in units of $2\pi/a$. The red (blue) lines indicate regions of high (low) transmission.

typically small values (hence *suppressed* instead of *zero* in the above rule). Second, the shape of the Fermi surface changes with the modifications being strongest in the vicinity of RL planes where, for Al, we observe the opening of gaps between previously connected fragments. The anisotropy is mostly related to this second effect.

In Fig. 2, we show the intersection of the Al FS with a (110) plane. The two plots are rotated so that the vertical axis in Fig. 2(a) is the [111] direction, while in Fig. 2(b) it is [001]. In both cases, the positions of the nearest RL sites (on which spheres are centered) are shown together with the cross section through the relevant interface-adapted Brillouin zone, which is different for each orientation; see Fig. 1(i). We can now readily identify spheres from which various fragments of the Fermi surface originate and mark those fragments with positive (upward) velocities, according to the rule given above, as having high (red) or low (blue) transmissions. In the (001) case, the ''high'' fragments originate from $(0, 0, 0)$ and $(0, 0, -2)$ centered spheres. Comparing Figs. 1(f) and 2(b), we note that the position of the gaps opened between these spheres by Bragg reflection on the (001) and $(00\bar{1})$ planes coincides, in projection along the [001] direction, with the position of the cold ring in Fig. 1(f). The other states present in this region originate from $(1, -1, -1)$ (and equivalent) centered spheres, are therefore nearly orthogonal to states in Ag centered on $(0, 0, 0)$, and so have low transmission. In the (111) case, however, the large fragments of FS belonging to the same $(1, -1, -1)$ sphere have high transmissions [Fig. 2(a)] and dominate transport. In addition, the gap-opening effect is reduced in this orientation because of the rotation. Combination of these two factors results in the almost uniformly high transmission seen in Fig. 1(c).

We can now finally identify the origin of the transmission anisotropy for the Al/Ag interface. It stems from two factors: (i) the near orthogonality of the downfolded Al states to those belonging to the simple Ag sphere and (ii) the gaps opened in the continuous free-electron Fermi surface by the periodic potential. The latter factor is, of course, related to the symmetry of the underlying crystal lattice and directly responsible for the introduction of the orientation dependence. For Al/Au interfaces, the interface transmissions and resistances are very similar to the Al/Ag case.

The orientation dependence of the interface transmission of six metal pairs with the same structure and lattice parameter was calculated. For fcc Ag/Al, a factor of 2 difference between the (111) and (001) orientations was found and explained within the free-electron model. The predicted anisotropic interface resistance and Andreev reflection (not shown) are not very sensitive to interface disorder and should be observable experimentally.

K. X. is supported by NSFC Grant No. 90303014 and CAS BRJH. This work is part of the research program of the ''Stichting voor Fundamenteel Onderzoek der Materie'' (FOM) and the use of supercomputer facilities was sponsored by the ''Stichting Nationale Computer Faciliteiten'' (NCF), both financially supported by the ''Nederlandse Organisatie voor Wetenschappelijk Onderzoek'' (NWO). It is also supported by ''NanoNed,'' a nanotechnology program of the Dutch Ministry of Economic Affairs. We are grateful to Anton Starikov for permission to use his sparse matrix version of the TB-MTO code.

*Permanent address: Institute of Molecular Physics, P.A.N., Smoluchowkiego 17, 60-179 Poznań, Poland.

[1] See the collection of articles in *Ultrathin Magnetic Structures I–IV*, edited by J. A. C. Bland and B. Heinrich (Springer-Verlag, Berlin, 1994–2005).
[2] K. M. Schep *et al.*, Phys. Rev. B **56**, 10 805 (1997).
[3] M. D. Stiles and D. R. Penn, Phys. Rev. B **61**, 3200 (2000).
[4] K. Xia *et al.*, Phys. Rev. B **63**, 064407 (2001).
[5] J. Bass and W. P. Pratt, Jr., J. Magn. Magn. Mater. **200**, 274 (1999).
[6] C. W. J. Beenakker, Rev. Mod. Phys. **69**, 731 (1997).
[7] C. Galinon *et al.*, Appl. Phys. Lett. **86**, 182502 (2005).
[8] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Holt-Saunders International Editions, Philadelphia, 1976).
[9] I. I. Mazin, Phys. Rev. Lett. **83**, 1427 (1999).
[10] I. I. Mazin, A. A. Golubov, and B. Nadgorny, J. Appl. Phys. **89**, 7576 (2001).
[11] M. Zwierzycki *et al.*, Phys. Rev. B **67**, 092401 (2003).
[12] K. Xia *et al.*, Phys. Rev. B **73**, 064420 (2006).
[13] G. E. Blonder, M. Tinkham, and T. M. Klapwijk, Phys. Rev. B **25**, 4515 (1982).
[14] R. J. Soulen, Jr. *et al.*, Science **282**, 85 (1998).
[15] S. K. Upadhyay *et al.*, Phys. Rev. Lett. **81**, 3247 (1998).
[16] O. K. Andersen, O. Jepsen, and D. Glötzel, in *Highlights of Condensed Matter Theory*, edited by F. Bassani, F. Fumi, and M. P. Tosi (North-Holland, Amsterdam, 1985), pp. 59–176.
[17] I. Turek, V. Drchal, J. Kudrnovský, M. Šob, and P. Weinberger, *Electronic Structure of Disordered Alloys, Surfaces and Interfaces* (Kluwer, Boston, 1997).
[18] Fe/Cr is an exception. For the majority spin channel, a large orientation dependence of the interface transmission is predicted. Unlike in the case of Al/Ag, this result is very sensitive to interface disorder. In addition, a single spin channel cannot be studied directly, making it difficult to obtain an unambiguous experimental result.
[19] We performed an extensive series of total energy calculations using local-density and generalized gradient approximations to relax the various Al/Ag interfaces. Only a small dependence of the interface energy on the orientation was found. The transport calculations were repeated using the resulting relaxed geometries. The effect on the interface transmission is less than 3%, which is negligible on the scale of the predicted factor of 2 orientation dependence.
[20] Moreover, the free-electron formula would lead to the violation of the unitarity of the scattering matrix (i.e., the conservation of particles) whenever there is more than one state on either side of the interface.