Possibility of observing spin-polarized electrons on the GaAs (110) surface with a scanning tunneling microscope

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A method is proposed for distinguishing the spin-dependent component of the tunneling current between a ferromagnetic tip and a GaAs (110) surface with spin-polarized electrons in a scanning tunneling microscope.

The scanning tunneling microscope (STM) is presently being used to manipulate individual atoms on surfaces,[1] to study the emission of photons during tunneling,[2] and to detect the precession of individual spins at paramagnetic centers.[3] The application of laser light to a tunneling gap makes it possible to study the dynamic tunneling characteristics[4] and resonantly excited surface modes (adsorbates and plasmons[5]). Photoexcitation of carriers in semiconductors during the scanning has made it possible to study the spectra and spatial distributions of nonequilibrium quasiparticles with a resolution at the atomic scale.[6,7]

If the tip in an STM is made of a magnetic material, it becomes possible to study the surface structure of magnetic materials. Ferromagnetic terraces with various magnetization orientations on a Cr (001) surface were observed in Ref. 8 with the help of a single-domain tip of ferromagnetic CrO_2. Recent experiments with a ferromagnetic tip of Fe have succeeded in revealing magnetic Fe^{3+} and Fe^{2+} ions on the (001) surface of the spinel Fe_3O_4 with a resolution genuinely at the atomic scale.[9]

A magnetic ordering of electron spins can be achieved in several III–V semiconductors through the interband absorption of circularly polarized light.[10,11] An STM with a magnetic tip opens up additional opportunities for studying the spin polarization of electrons with a resolution at the atomic scale.

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When circularly polarized light is applied to GaAs in a steady-state fashion, a nonequilibrium carrier distribution and an associated spin polarization arise because of the particular features of the band structure.[10,11] It follows from the experiments of Refs. 6 and 7 that the tunneling current is dominated by the nonequilibrium distribution function in the semiconductor. We also believe that in the case of a weak tunneling coupling the tunneling occurs against the backdrop of a nonequilibrium distribution function, whose distortion by the tunneling can be ignored. The dynamic effect related to the modulation of the barrier height is important for only certain materials, e.g., graphite.[4]

Since the crystal-tip system does not have translational invariance, we use a basis of localized orbitals $|\varphi_{n\sigma}(\vec{r}-\vec{R}_l)\rangle$, i.e., an orbital of type $n(s,p,d,...)$ with a spin σ at site $\vec{R}_l$.

We can write the tunneling current in terms of Keldysh Green's functions as follows,[12] within terms up to T^2:

$$I = \frac{e}{\hbar}\mathrm{TR}\{\int \frac{d\epsilon}{2\pi i}[\hat{T}\hat{g}_c^+(\epsilon)\hat{T}^*\hat{g}_t^-(\epsilon) - \hat{T}^*\hat{g}_c^-(\epsilon)\hat{T}\hat{g}_t^+(\epsilon)]\}, \quad (1)$$

where $\hat{g}_{c,t}^{\pm}(\epsilon)$ are Green's functions which are matrices in terms of the orbital, site, and spin indices. The tunneling coupling between the tip and the crystal is described by an overlap matrix which is diagonal in the spin:

$$\hat{T} = \{T_{n'l'}^{nl}\} = \frac{i\hbar}{2m}\int ds[\varphi_{n\sigma}(\vec{r}-\vec{R}_l)\frac{\vec{d}}{d\vec{r}}\varphi_{n'\sigma}^*(\vec{r}-\vec{R}_{l'}) - \mathrm{H.a.}]. \quad (2)$$

We are left with the problem of determining $\hat{g}_{c,t}^{\pm}$ for a crystal and a tip which are not interacting with each other, in the case of a spin polarization.

The magnetization in a semiconductor is distinguished in a fundamental way because of the illumination and the ferromagnetic tip: In the tip, at thermodynamic equilibrium, the distribution of carriers between the spectral branches with different spin orientations is described by a common Fermi distribution function. The densities of states in the different spin subbands are different in this case. In the semiconductor, the densities of states in the subbands with moment projections up and down are identical (effects stemming from the absence of a center of inversion at the surface of a III–V compound are minor[13]), but the distribution functions of the quasiparticles with different moment projections are different. The distribution function in a metal may also be a nonequilibrium distribution; the only point of importance is that this distribution is not spin-polarized. A nonequilibrium distribution function could be spin-polarized only because of particular features of the band structure, as in GaAs.

The Keldysh Green's functions for a semiconductor in the representation which is diagonal for the quasiparticles are

$$\hat{g}_{\mu m}^{\mu m}(\epsilon) = <\psi_{\mu m}|\hat{g}^{\pm}|\psi_{\mu m}^*> = 2\pi i\delta(\epsilon-\epsilon_{\mu m})\begin{cases} f_m(\epsilon) \\ f_m(\epsilon)-1 \end{cases}, \quad (3)$$

where m specifies the moment projection ($m = \pm 1/2, \pm 3/2$), μ represents the set of other quantum numbers (the quasimomentum along the surface and the band index), and f_m is the distribution function of quasiparticles in the band with moment projection m. Since there are no surface states at the GaAs (110) surface,[14] the $\psi_{\mu m}$ describe states in the continuous spectrum with an energy $\epsilon_{\mu m}$.

Going over to a nondiagonal basis of localized orbitals, in which the tunneling current is expressed, we find

$$\hat{g}^{\pm}_{\substack{nl\sigma\\ n'l'\sigma'}}(\epsilon) =< \varphi_{n\sigma}(\vec{r}-\vec{R}_l)|\hat{g}^{\pm}(\epsilon)|\varphi^{*}_{n'\sigma}(\vec{r}-\vec{R}_{l'}) >$$

$$= 2\pi i \sum_{\mu m} A^{nl\sigma}_{\mu m}\delta(\epsilon-\epsilon_{\mu m})\, \overset{*\,n'l'\sigma'}{A_{\mu m}} \left\{ \begin{array}{c} f_m(\epsilon) \\ f_m(\epsilon)-1 \end{array} \right\}, \tag{4}$$

where $\hat{A}$ is the matrix which expands the eigenvectors in the localized orbitals:

$$|\psi_{\mu m} >= \sum_{\mu m} A^{nl\sigma}_{\mu m}|\varphi_{n\sigma}(\vec{r}-\vec{R}_l) > . \tag{5}$$

If the distribution function does not depend on the projection index m, $\hat{g}^{\pm}$ becomes

$$\hat{g}^{\pm}_{\substack{nl\sigma\\ n'l'\sigma'}}(\epsilon) = 2\pi i \rho_{\substack{nl\sigma\\ n'l'\sigma'}}(\epsilon) \left\{ \begin{array}{c} f(\epsilon) \\ f(\epsilon)-1 \end{array} \right\}, \tag{6}$$

where the partial density of states is

$$\rho_{\substack{nl\sigma\\ n'l'\sigma'}}(\epsilon) = \sum_{\mu m} A^{nl\sigma}_{\mu m}\delta(\epsilon-\epsilon_{\mu m})\, \overset{*\,n'l'\sigma'}{A_{\mu m}} . \tag{7}$$

For the tip in the spin-polarized case, $\hat{g}^{\pm}$ can be written as follows [the caret (^) here refers to the spin indices]:

$$\hat{g}^{\pm}_{\substack{nl\sigma\\ n'l'\sigma'}}(\epsilon) = 2\pi i(\hat{\rho}^{nt}_{\substack{nl\\ n'l'}}(\epsilon) + \hat{\rho}^{st}_{\substack{nl\\ n'l}}(\epsilon)(\hat{\vec{\sigma}}\vec{n}_t)) \left\{ \begin{array}{c} f(\epsilon) \\ f(\epsilon)-1 \end{array} \right\}, \tag{8}$$

where $\hat{\rho}^{n,st}$ are the spin-independent and spin-dependent parts of the density of states, $\vec{n}_t$ is the magnetization direction in the tip (we assume for simplicity that the tip is in a single-domain state and that $\vec{n}_t$ does not depend on the angle), and the index t means "tip."

For a semiconductor in the nondiagonal representation, we cannot factorize $\hat{g}^{\pm}$ into the product of the density of states and the distribution function because of the dependence of the distribution function on the moment projection. Taking this point into account in the spin-polarized case, singling out the normal part F^n and the spin-polarized part F^s of the density matrix in (4), we find

$$\hat{g}^{\pm}_{\substack{nl\sigma\\ n'l'\sigma'}}(\epsilon) = 2\pi i \left\{ \hat{F}^{nc}_{\substack{nl\\ n'l'}}(\epsilon) + \hat{F}^{sc}_{\substack{nl\\ n'l'}}(\epsilon)(\hat{\vec{\sigma}}\vec{n}_c)) - \left[\hat{\rho}^{c}{}^{0}_{\substack{nl\\ n'l'}}(\epsilon) \quad \delta_{\sigma\sigma'} \right] \right\}, \tag{9}$$

where $\vec{n}_c$ is the magnetization direction in the GaAs. This direction is determined by the illumination conditions. The superscript c means "crystal."

Using (1), (8), and (9), we find the following expression for the tunneling current:

$$I^{\pm} = I^{\pm}_n \pm I^{\pm}_s = \frac{2\pi e}{\hbar}\mathrm{Tr}\{\int d\epsilon[\hat{T}\hat{\rho}^{c}(\epsilon)\hat{T}^{*}\hat{\rho}^{nt}(\epsilon)f(\epsilon) - \hat{T}^{*}\hat{\rho}^{nt}(\epsilon)\hat{T}^{*}\hat{F}^{nc}(\epsilon)]$$

$$\pm(\vec{n}_c\vec{n}_t)\hat{T}\hat{F}^{cs}(\epsilon)\hat{T}^{*}\hat{\rho}^{st}(\epsilon)\}. \tag{10}$$

We have singled out the spin-dependent part of the current, I_s, only in a formal sense here; the $\pm$ corresponds to right-hand and left-hand circular polarization of the light. The spin part of the density matrix of a semiconductor changes sign (the magnetization does also) when the sense of the circular polarization is reversed, so we can write

$$I^{+}_s - I^{-}_s = (\vec{n}_c\vec{n}_t)\frac{4\pi e}{\hbar}\mathrm{Tr}\{\int d\epsilon \hat{\mathrm{T}}\hat{\mathrm{F}}^{cs}(\epsilon)\hat{\mathrm{T}}^{*}\hat{\rho}^{st}(\epsilon)\}. \tag{11}$$

We could also have derived expression (11) on the basis of qualitative considerations. To show this, we assume that the magnetization in the crystal and that in the tip are in the same direction. The contribution from spin-up electrons satisfies

$$I_{\uparrow} \propto \int d\epsilon\{\rho(\epsilon)\rho_{\uparrow}(\epsilon)[f(\epsilon)[1 - f_{\uparrow}(\epsilon)] - f_{\uparrow}(\epsilon)[1 - f(\epsilon)]\},$$

and that from spin-down electrons satisfies

$$I_{\downarrow} \propto \int d\epsilon\{\rho(\epsilon)\rho_{\downarrow}(\epsilon)[f(\epsilon)[1 - f_{\downarrow}(\epsilon)] - f_{\downarrow}(\epsilon)[1 - f(\epsilon)]\}, \tag{12}$$

where $f_{\uparrow\downarrow}, f$ and $\rho(\epsilon), \rho_{\uparrow\downarrow}(\epsilon)$ are the nonequilibrium distribution function and the density of states in the semiconductor and the tip, respectively. For a given sense of the circular polarization the total current is

$$I^{+} = I_{\uparrow} + I_{\downarrow} \propto \int d\epsilon \left\{ \frac{1}{2}\rho(\epsilon)[(\rho_{\downarrow}(\epsilon) + \rho_{\uparrow}(\epsilon))[f - (f_{\uparrow} + f_{\downarrow})/2]]\right.$$

$$\left. + \frac{1}{2}\rho(\epsilon)[(\rho_{\downarrow}(\epsilon) - \rho_{\uparrow}(\epsilon))[f - (f_{\uparrow} - f\downarrow)/2]]\right\}. \tag{13}$$

When the sense of the circular polarization is reversed, the distribution functions in the semiconductor for the spin-up and spin-down cases trade places ($f_{\uparrow\downarrow} \rightleftharpoons f_{\downarrow\uparrow}$). The densities of states $\rho_{\uparrow}$ and $\rho_{\downarrow}$ in the tip obviously do not change, so we have

$$I^+ - I^- \propto \int d\epsilon\rho(\epsilon)[(\rho_\downarrow(\epsilon) - \rho_\uparrow(\epsilon)[f_\uparrow - f_\downarrow], \tag{14}$$

which is essentially the same as (11). The difference between the currents in (14) does not depend on the nonequilibrium distribution function in the tip. We thus also conclude that the initial partitioning of the current into I_n and I_s in (10) was somewhat arbitrary.

We conclude with a discussion of the implications for the GaAs (110) surface. When the positive voltage is applied to the test sample, the tunneling occurs mostly to states in the conduction band. In this case the maximum current is observed when the tip is positioned above a Ga atom, since the orbitals of this atom (primarily the s-type orbital) shape the edge of the conduction band. By varying the angle of incidence of the light and measuring the tunneling current for a given angle of incidence, but for different polarization directions, one can cause the combination $I^+ - I^- \propto (\vec{n}_c\vec{n}_t)$ to vanish at some angle (and thus at some direction of the photon spin and of the magnetization in the GaAs). This circumstance can be exploited to determine the orientation of the magnetization at the end of the tip. The tunneling of holes out of the valence band will be suppressed in this case if the tip is above a Ga atom, since the states at the edge of the valence band are localized at As atoms. This circumstance is responsible for the differences in the tunneling contrast for different polarities of the applied voltage.[14] If the negative voltage is applied to the sample, and if the tip is positioned above an As atom, there should be no dependence of the tunneling current on the angle of incidence or the direction of the polarization, since there will be no spin ordering of the holes.[10,11] When the tip is moved to a position above a Ga atom, one should observe a current signal which depends on the illumination because of a possible tunneling of nonequilibrium spin-polarized electrons.

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