Ideal spin filters: A theoretical study of electron transmission through ordered and disordered interfaces between ferromagnetic metals and semiconductors

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It is predicted that certain atomically ordered interfaces between some ferromagnetic metals (F) and semiconductors (S) should act as ideal spin filters that transmit electrons only from the majority spin bands or only from the minority spin bands of the F to the S (and from the S only to the majority spin bands or only to the minority spin bands of the F) at the Fermi energy, even for F with both majority and minority bands at the Fermi level. Criteria for determining which combinations of F, S, and interface should be ideal spin filters are formulated. The criteria depend only on the bulk band structures of the S and F and on the translational symmetries of the S, F, and interface. Several examples of systems that meet these criteria to a high degree of precision are identified. Disordered interfaces between F and S are also studied and it is found that intermixing between the S and F can result in interfaces with spin antifiltering properties, the transmitted electrons being much *less* spin polarized than those in the ferromagnetic metal at the Fermi energy.

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I. INTRODUCTION

In ferromagnetic condensed matter systems the spin up and spin down states are occupied asymmetrically by electrons. Because of this asymmetry, it is possible for an applied electric field to drive a spin-polarized electron current across the interface between a ferromagnet and a nonmagnetic material. Spin-polarized electron transport has been achieved experimentally from ferromagnetic metals to superconductors by Meservey, Tedrow, and Fulde,[1] from ferromagnetic to normal metals by Johnson and Silsbee,[2] between ferromagnetic metals separated by thin insulating films by Julliere,[3] and from magnetic semiconductors to nonmagnetic semiconductors by Fiederling *et al.*[4] and Ohno *et al.*[5]

Injection of strongly spin-polarized electron currents from ferromagnetic metals into semiconductors has also long been recognized as an important fundamental goal in condensed matter physics.[6] Attaining it would have a significant technological impact in the area of spintronics, the branch of electronics that utilizes the electron's spin degree of freedom as well as its charge to store, process, and transmit information. However, only weak signatures of the spin polarization of electrons injected from ferromagnetic metals into semiconductors through the metal-semiconductor interface have been reported[7,8] and the interpretation of such experiments is controversial.[9–11]

By extending previous theoretical work by van Son, van Kempen, and Wyder[12] and by Valet and Fert[13] on spin transport in metallic systems, Schmidt *et al.*[14] recently concluded that for devices in the diffusive transport regime only a weak ($<0.1\%$) spin polarization of electrons injected from a ferromagnetic metal into a semiconductor is possible, even in principle, unless the ferromagnetic contact is almost 100% spin polarized, which is not the case for such common ferromagnetic metals as Fe, Co, Ni, and Permalloy. The essential reason was that in an electric circuit consisting of a diffusive semiconductor in series with a metal, the net resistance of the circuit is dominated by the resistance of the semiconductor which is spin independent, and therefore the spin up and down currents flowing through the semiconductor should be almost equal. However, Schmidt *et al.*[14] did not allow in their analysis for the possibility that electron transmission through the interface between the ferromagnet and semiconductor may be very strongly spin dependent.

In this article the spin dependence of electron transmission from ferromagnetic metals to semiconductors is examined theoretically. It is predicted that, in contrast to the interfaces between ferromagnetic and normal metals and to the tunnel barriers between ferromagnetic metals previously discussed in the literature,[15–20] atomically ordered and suitably oriented interfaces between some ferromagnetic metals and some semiconductors should be *almost perfect spin filters*. That is, they should transmit only majority or only minority spin band electrons from the ferromagnet to the semiconductor even for ferromagnetic metals for which both majority and minority spin bands are present at the Fermi level. Such spin filters make it possible, in principle, to overcome the difficulties discussed by Schmidt *et al.*[14] and to achieve injection of strongly spin-polarized electric currents from ferromagnetic metals into semiconductors. Several examples of combinations of ferromagnetic metals, semiconductors, and interfaces that are good candidates for near-ideal spin filters are identified in this article.

Recently it has been proposed by Ferreira *et al.* that a superlattice that consists of alternating layers of two different materials arranged in a periodic sequence may be a perfect spin filter for electron transmission between two ferromagnets[21] and that a pair of magnetic superlattices connected by a conducting medium with a low carrier density may also be a perfect spin filter.[22] These possibilities were explored using simple free electron models and Kronig-Penney-like potentials.[21,22] By contrast the ideal spin filters introduced here require only a *single* interface for their operation and the spin-polarized electron transmission is between a ferromagnet and semiconductor. Also the present work takes into account the atomic crystal structures and realistic electronic band structures of the materials involved.

The present approach to injecting spin-polarized electrons from ferromagnetic metals into semiconductors also differs fundamentally from a previous suggestion by Johnson[23,11] that was based on the Rashba effect in quasi-two-dimensional electron gases.

The effects of disorder at the interface on the spin polarization of electrons transmitted from ferromagnetic metals to semiconductors are also addressed in the present work by solving a simple tight-binding model numerically. The model exhibits perfect spin filtering for an ordered interface between the semiconductor and ferromagnetic metal. Intermixing between the semiconductor and metal at the interface drastically reduces the spin polarization of the transmitted electron flux. When intermixing completely destroys the interface symmetries that result in spin filtering, the spin polarization of the transmitted electron flux does not resemble that of the ferromagnetic metal at the Fermi level; it is very much weaker. This effect has a different physical origin from that discussed by Schmidt *et al.*[14]

The article is organized as follows: In Sec. II general selection rules for electron transmission through atomically ordered interfaces between crystals are derived in a form suited to the present purpose. Criteria for identifying possible candidates for ideal spin filters are then formulated based on these selection rules.

The selection rules derived in Sec. II are exact and apply not only to interfaces between ferromagnetic metals and semiconductors (the subject of the present work) but also to ordered interfaces between crystalline materials in general. Theoretical work on electron transmission through the ordered interfaces between various crystalline materials, based on *ab initio* computer calculations and analytic models, has been published by several authors.[15–22,24,25] The general form of the selection rules that is derived in Sec. II and is needed for the present purpose does not appear in those publications but is consistent with the formalism underlying the *ab initio* calculations.

In Sec. III some examples of combinations of ferromagnetic metals, semiconductors, and interfaces that are candidates for nearly ideal spin filters are identified and discussed. The effects of disorder at the interface on the spin polarization of the transmitted current are examined in Sec. IV. A summary and some further comments are contained in Sec. V.

II. SELECTION RULES AND CRITERIA FOR IDEAL SPIN FILTERS

When an electron is transmitted through an ordered interface between two crystals, the projection of its Bloch state wave vector onto the interface is conserved up to reciprocal lattice vectors. In this section, I derive a precise formulation of this principle that applies to electron transmission through general semiconductor-ferromagnetic metal interfaces. Based on this formulation, I then define criteria for identifying combinations of ferromagnetic metals, semiconductors, and interfaces that are candidates for ideal spin filters.

Consider an atomically ordered plane interface between two crystals, a semiconductor S and a ferromagnetic metal M. The two crystals may be in direct contact with each other at the interface or the interface may include one or more ordered layers of other atomic species than those present in S and M and/or the same species in a different spatial arrangement.

Far from the interface the periodicities of the two crystals are described by their three-dimensional sets of Bravais lattice vectors $\{\mathbf{R}_S\}$ and $\{\mathbf{R}_M\}$, respectively. The periodicity of the entire system consisting of the two crystals and the interface is described by a two-dimensional Bravais lattice of symmetry translations $\{\mathbf{R}_I\}$ parallel to the plane of the interface. The corresponding three and two-dimensional reciprocal lattices are the sets of vectors $\{\mathbf{K}_S\}$, $\{\mathbf{K}_M\}$, and $\{\mathbf{K}_I\}$, respectively.

Because of the symmetry of the entire system under the set of translations $\{\mathbf{R}_I\}$ parallel to the plane of the interface, a complete set of one-electron energy eigenstates of the entire system can be chosen in the Bloch form

$$\Psi_{\mathbf{k}_I s}(\mathbf{r}) = e^{i\mathbf{k}_I\cdot\mathbf{r}} u_{\mathbf{k}_I s}(\mathbf{r}), \tag{1}$$

where $\mathbf{r}$ is the position of the electron, $\mathbf{k}_I$ is a vector parallel to the plane of the interface, and u can be written in the form $u_{\mathbf{k}_I s}(\mathbf{r}) = \Sigma_{\mathbf{K}_I} \Lambda^{\mathbf{k}_I s}_{\mathbf{K}_I}(\mathbf{r}_\perp) e^{i\mathbf{K}_I\cdot\mathbf{r}}$. Here the Fourier coefficients $\Lambda^{\mathbf{k}_I s}_{\mathbf{K}_I}$ depend on $\mathbf{r}_\perp$, the component of $\mathbf{r}$ in the direction orthogonal to the plane of the interface. The states $\Psi_{\mathbf{k}_I s}$ include among them the scattering states of electrons that are incident on the interface from the ferromagnetic metal crystal at the Fermi energy and are partly or completely transmitted and/or reflected at the interface. Deep in the ferromagnet these scattering states can be written as linear combinations of the Bloch states $\psi_{\mathbf{k}_M \tilde{s}}$ of the [three-dimensional (3D)] ferromagnetic metal crystal at the Fermi energy. I.e., deep in the ferromagnet,

$$\Psi_{\mathbf{k}_I s}(\mathbf{r}) = \sum_{\mathbf{k}_M, \tilde{s}} A^{\mathbf{k}_I s}_{\mathbf{k}_M \tilde{s}} \psi_{\mathbf{k}_M \tilde{s}}(\mathbf{r}). \tag{2}$$

Writing the Bloch states $\psi_{\mathbf{k}_M \tilde{s}}$ of the ferromagnet in the Fourier form $\psi_{\mathbf{k}_M \tilde{s}}(\mathbf{r}) = \Sigma_{\mathbf{K}_M} \lambda^{\mathbf{k}_M \tilde{s}}_{\mathbf{K}_M} e^{i(\mathbf{k}_M + \mathbf{K}_M)\cdot\mathbf{r}}$ and combining Eq. (1) with Eq. (2) then yields

$$\sum_{\mathbf{K}_I} \Lambda^{\mathbf{k}_I s}_{\mathbf{K}_I}(\mathbf{r}_\perp) e^{i(\mathbf{k}_I + \mathbf{K}_I)\cdot\mathbf{r}} = \sum_{\mathbf{k}_M, \mathbf{K}_M, \tilde{s}} A^{\mathbf{k}_I s}_{\mathbf{k}_M \tilde{s}} \lambda^{\mathbf{k}_M \tilde{s}}_{\mathbf{K}_M} e^{i(\mathbf{k}_M + \mathbf{K}_M)\cdot\mathbf{r}} \tag{3}$$

for $\mathbf{r}$ deep in the ferromagnet. Equation (3) can only be satisfied for all $\mathbf{r}$ deep in the ferromagnet if for some $\mathbf{k}_M$ on the ferromagnet's Fermi surface and for some reciprocal lattice vectors $\mathbf{K}_I$ and $\mathbf{K}_M$:

$$\mathbf{k}_I = (\mathbf{k}_M + \mathbf{K}_M)_\parallel - \mathbf{K}_I, \tag{4}$$

where $(\cdots)_\parallel$ denotes projection onto the plane of the interface. Similarly, deep in the semiconductor the same scattering states can be expressed in terms of semiconductor Bloch states yielding instead of Eq. (4)

$$\mathbf{k}_I = (\mathbf{k}_S + \mathbf{K}_S)_\parallel - \mathbf{K}_I' , \tag{5}$$

where $\mathbf{k}_S$ is a vector on the Fermi surface of the semiconductor and $\mathbf{K}_I'$ is a vector of the two-dimensional reciprocal lattice of the entire system. For transmission from the ferromagnet to the semiconductor to occur, both Eqs. (4) and (5) must be satisfied and thus

$$(\mathbf{k}_S)_\parallel = (\mathbf{k}_M)_\parallel + (\mathbf{K}_M - \mathbf{K}_S)_\parallel - \mathbf{K}_I + \mathbf{K}_I' . \tag{6}$$

Let the word ''projection'' stand for ''projection onto the plane of the interface.'' Then Eq. (6) implies the following selection rule: Transmission of electrons at the Fermi energy is forbidden from the majority (minority) spin bands of the ferromagnet to the semiconductor (and vice versa) unless the projections of the Fermi surfaces of the semiconductor and of the majority (minority) spin bands of the ferromagnetic metal are connected by a vector that is the sum of a (2D) reciprocal lattice vector of the entire system and projections of reciprocal lattice vectors of the semiconductor and ferromagnet.

It should be noted that the above selection rule depends only on the bulk electronic structure of the ferromagnetic metal and semiconductor and on translational symmetries, and not on the details of the electronic structure of the interface.

If in this way transmission of majority spin band electrons from the ferromagnet to the semiconductor is allowed but that of minority spin band electrons is forbidden (or vice versa), then, in the absence of spin-flip scattering and if spin-orbit coupling can be neglected (see Sec. V), the system is an ideal spin filter for injection of spin-polarized electrons from the ferromagnet into the semiconductor.

While the above derivation of the criteria for ideal spin filters also applies to interfaces between normal and ferromagnetic metals, the Fermi surfaces of most metals enclose large enough fractions of the Brillouin zone that the criteria cannot be satisfied. On the other hand, the Fermi surface of a semiconductor encloses only a very small fraction of the Brillouin zone. Because of this, some combinations of ferromagnetic metal, semiconductor, and interface are possible candidates for nearly ideal spin filters as will be seen below.

III. SOME CANDIDATES FOR NEARLY IDEAL SPIN FILTERS

A. Simplest case

The simplest semiconductors to consider in the present context are those with a single lowest conduction band minimum (for *n*-type materials) or highest valence band maximum (for *p*-type materials[26]) located at the center of the Brillouin zone (i.e., at $\mathbf{k}=0$) so that $(\mathbf{k}_S)_\parallel = 0$ in Eq. (6).

For such semiconductors it is helpful to examine separately the case where $(\mathbf{K}_M)_\parallel = (\mathbf{K}_S)_\parallel = \mathbf{K}_I = \mathbf{K}_I' = 0$ in Eq. (6) so that Eq. (6) reduces to

$$(\mathbf{k}_M)_\parallel = 0 \tag{7}$$

and the complimentary case where one or more of $(\mathbf{K}_M)_\parallel$, $(\mathbf{K}_S)_\parallel$, $\mathbf{K}_I$, and $\mathbf{K}_I'$ is not zero so that Eq. (6) becomes

$$(\mathbf{k}_M)_\parallel = \mathbf{K}_I - \mathbf{K}_I' - (\mathbf{K}_M - \mathbf{K}_S)_\parallel . \tag{8}$$

The criteria for ideal spin filters derived in Sec. II then reduce to the following.

(1) Neither Eq. (7) nor Eq. (8) should be satisfied (for any choice of $\mathbf{K}_M$, $\mathbf{K}_S$, $\mathbf{K}_I$, and $\mathbf{K}_I'$) for any $\mathbf{k}_M$ on the majority (minority) spin Fermi surface of the metal.

(2) Either Eq. (7) or Eq. (8) (for some choice of $\mathbf{K}_M$, $\mathbf{K}_S$, $\mathbf{K}_I$, and $\mathbf{K}_I'$) or both should be satisfied for some $\mathbf{k}_M$ on the minority (majority) spin Fermi surface of the metal.

Whether Eq. (7) is satisfied depends only on the Fermi surface geometry of the metal and the orientation of the interface but *not* on the crystal structure of the semiconductor, metal, or interface. This greatly simplifies the process of screening for systems involving direct gap semiconductors that may be nearly ideal spin filters: Start by identifying as possible candidates those combinations of ferromagnetic metal and interface orientation for which Eq. (7) is *not* satisfied for the majority spin Fermi surface, the minority spin Fermi surface, or both. Having narrowed the field of potential candidates in this way, proceed with detailed analyses of the crystal structures of specific combinations of materials at suitably oriented interfaces to determine whether the remaining conditions for ideal spin filters that involve Eqs. (8) and (7) are also satisfied.

Inspection of the calculated band structures and Fermi surfaces of some common ferromagnetic metals that are available in the literature[27–29] shows that Eq. (7) is not satisfied for the majority spin Fermi surface of hcp Co if the interface is orthogonal to the (001) crystallographic axis, i.e., parallel to a basal plane of hexagonally close-packed Co atoms. This is also the case for fcc Ni and fcc Co for interfaces perpendicular to their (111) crystallographic axes.[30] Some other ferromagnetic metals whose published electronic band structures[29,31–36] also do not satisfy Eq. (7) for majority and/or minority spin electrons and some orientation(s) of a putative interface plane include simple cubic Mn, CoS_2, FeAl, τ-MnAl, Gd, Tb, and some magnetic superlattices.

While consideration of Eq. (7) can be a useful starting point, a more detailed analysis of specific systems consisting of the ferromagnetic metal, semiconductor, and interface is essential to determine whether they satisfy *all* of the criteria for ideal spin filters derived in Sec. II. Such analyses will be outlined below for a number of systems involving the ferromagnetic metals Co, Ni, CoS_2, FeAl, τ-MnAl, Gd, Tb, Pd_3Fe, Co_3Pt, and some magnetic superlattices together with a variety of *n*- and *p*-type direct and indirect gap semiconductors.

B. Spin filters involving the ferromagnetic metals hcp Co, fcc Ni, or fcc Co

1. Semiconductors with Fermi surfaces at the center of the first Brillouin zone

The (001) crystallographic planes of hcp Co and the (111) planes of fcc Ni and fcc Co consist of metal atoms in a hexagonal close-packed arrangement. The (111) atomic planes of semiconductors with the diamond and zinc blende crystal structure also have hexagonal atomic arrangements,

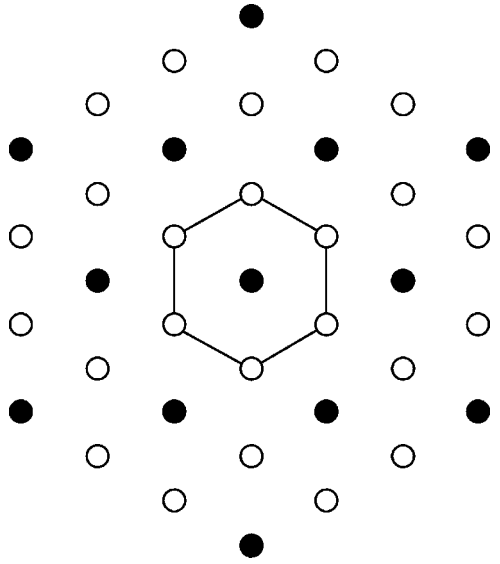

FIG. 1. Schematic of reciprocal lattice vectors and projections of reciprocal lattice vectors onto the plane of the interface that enter Eq. (6) for interfaces between hcp Co, fcc Ni, and fcc Co and semiconductors with the diamond, zinc blende, and wurtzite structures that are perfectly matched to these metals as described in the text. Projections of the reciprocal lattice vectors of the metal onto the interface plane are represented by solid circles. The projections of the reciprocal lattice vectors of the semiconductor are indicated by both open and solid circles. The open and solid circles also indicate the reciprocal lattice vectors that are associated with the group of symmetry translations (parallel to the interface plane) of the whole system consisting of the two crystals and the interface between them. The hexagon is the projection of the boundary of the first Brillouin zone of hcp Co onto the interface plane.

but in most cases with considerably larger in-plane nearest-neighbor atomic spacings than those of the metals. Direct gap semiconductors with the wurtzite structure also have planes of atoms in a hexagonal arrangement, and the in-plane nearest-neighbor spacings are again in most cases significantly larger than those of the metals. However, for many of these semiconductors, these in-plane nearest-neighbor atomic spacings are larger than those in the metals by factors close to $\sqrt{3}$. For such semiconductors approximate atomic registry between the hexagonal atomic planes of the metal and semiconductor can be achieved by a rotation of the metal Bravais lattice relative to that of the semiconductor through a 30° angle about the axis perpendicular to the plane of the interface.

The reciprocal lattice vectors and projections of reciprocal lattice vectors onto the plane of the interface that enter Eq. (6) are shown schematically in Fig. 1 for interfaces between hcp Co, fcc Ni, and fcc Co, and semiconductors with the diamond, zinc blende, and wurtzite structures that are perfectly lattice matched to the metals as described in the preceding paragraph. The projections onto the plane of the interface of the reciprocal lattice vectors of the metals are represented by the solid circles. The projections onto the plane of the interface of the reciprocal lattice vectors of the semiconductors matched to the metals are indicated by both the open and solid circles. The open and solid circles also indicate the reciprocal lattice vectors that are associated with the group of symmetry translations (parallel to the interface plane) of the whole system consisting of the two crystals and the interface between them, assuming that no lattice reconstruction occurs at the interface. The hexagon (shown for reference) is the boundary of the projection of the first Brillouin zone of hcp Co onto the interface plane. For a direct gap semiconductor whose conduction band minimum (valence band maximum) is located at the center of the Brillouin zone, the open and solid circles also indicate the locations of the replicas of the conduction band minimum (valence band maximum) in the repeated zone scheme. Inspection of the calculated band structures and Fermi surfaces of hcp Co, fcc Ni, and fcc Co (Refs. 27–29), shows that the projection of the Fermi surface of the majority spin electrons in each of these metals onto the interface plane does not overlap any of these replicas of the semiconductor conduction band minimum (valence band maximum), whereas this is not true of the Fermi surfaces of the minority spin electrons. Therefore according to the reasoning in Sec. II only minority spin band electrons can be transmitted through the interface at the Fermi energy and the interface is an ideal spin filter if the semiconductor is perfectly lattice matched to the metal in the above sense.[30] [Note that consideration of Eq. (7) is by itself *not* sufficient to determine whether these systems should be ideal spin filters since Eq. (7) does not address whether the projections of the majority or minority Fermi surfaces of the metals onto the interface plane overlap the projections of the semiconductor reciprocal lattice vectors marked by open circles in Fig. 1; in an analysis based on the form of the theory described in Sec. III A, Eq. (8) must be considered as well.]

Some direct gap semiconductors with the zinc blende and wurtzite structure that approximately lattice match the metals in the above sense (and therefore are candidates for spin filters when either *n* or *p* doped) are listed below. In each case the name of the semiconductor is followed in parentheses by the ratio a_p/a (for hcp Co, fcc Ni, and fcc Co, respectively) of the value a_p of the lattice parameter required for a perfect match with the metal to the actual value a of the lattice parameter for the semiconductor.

Semiconductors with the zinc blende structure are ZnTe (1.006, 1.000, 1.006), GaSb (1.007, 1.001, 1.007), InAs (1.014, 1.008, 1.013); CdSe (1.015, 1.009, 1.014), CuI (1.016, 1.010, 1.016), InP (1.046, 1.040, 1.046); InSb (0.948, 0.942, 0.947), CdTe (0.947, 0.941, 0.946), CdS (1.054, 1.048, 1.054); ZnSe (1.083, 1.077, 1.083), GaAs (1.086, 1.080, 1.086).

Semiconductors with the wurtzite structure are CdSe (1.010, 1.004, 1.010), CdS (1.050, 1.044, 1.049).

An indirect gap semiconductor with zinc blende structure whose valence band maximum is at the center of the Brillouin zone is AlSb (1.001, 0.995, 1.000). As a *p*-type semiconductor it is also a potential spin filter in conjunction with the same metals.

For an interface to function as a nearly ideal spin filter, an accurate lattice match is clearly desirable. In the above list the accuracy of the lattice matching varies from excellent to marginal, depending on the materials involved. It may be

improved by alloying different semiconductors, for example, GaSb or InAs with InSb, at the expense of introducing random defects. There is reason to expect that in at least some cases such defects will not severely degrade the performance of spin filters (which depends on the conservation of projected Bloch state wave vectors up to reciprocal lattice vectors at the interface) since there exist heterostructures such as $GaAs/Al_xGa_{1-x}As$ in which a 2D electron gas can have very high mobilities despite being in contact with such a semiconductor alloy. Another way to improve the lattice matching is to grow very thin films (of the metal on the semiconductor or of the semiconductor on the metal) in which the metal and semiconductor are in perfect atomic registry with each other at the interface although the thin film is elastically strained.

2. Hexagonal boron nitride

The above examples have been of spin filters based on semiconductors whose relevant conduction band minimum or valence band maximum is located at the center of the Brillouin zone. However, the selection rules and criteria for ideal spin filters developed in Sec. II also apply to interfaces between ferromagnetic metals and semiconductors with relevant band extrema that are not at the Brillouin zone center.

Such an indirect gap semiconductor that satisfies the criteria for spin filters in conjunction with some ferromagnetic metals is hexagonal boron nitride [*h*-BN]. It has a layered structure (resembling graphite) with a hexagonal Bravias lattice. Its in-plane lattice parameter of 2.504 Å is a very good match to the nearest-neighbor distances 2.507, 2.492, and 2.506 Å in the hexagonal atomic layers of hcp Co, fcc Ni, and fcc Co, respectively. Because of this accurate lattice matching, monolayers of hexagonal boron nitride grown on (111) surfaces of fcc Ni are highly ordered and in atomic registry with the substrate.[37] Because BN consists of light atoms, the effects of spin-orbit coupling in BN should be very weak, which should be advantageous in a candidate for an ideal spin filter; see Sec. V.

For fcc and hcp crystals in *exact* atomic registry at the interface with a hexagonal basal plane of *h*-BN, the projections of the reciprocal lattice vectors of the fcc and hcp crystals onto the interface coincide with the projections of the *h*-BN reciprocal lattice vectors onto the interface and are indicated by the solid circles in Fig. 2. The projections of the first Brillouin zones of the hcp crystal and of *h*-BN onto the interface are indicated by the hexagon in the figure. Recent band structure calculations[38–40] indicate that *h*-BN is an indirect gap semiconductor with the lowest conduction band minimum at *M* and the valence band maximum at *H* or *K*. Combining these results with those in the literature[27–29] for the band structures and Fermi surfaces of hcp Co, fcc Ni, and fcc Co and applying the criteria developed in Sec. II yields the following predictions.

The interface between a hexagonal atomic layer of hcp Co and a hexagonal basal plane of *h*-BN should be a near ideal spin filter for both *n*-type and *p*-type *h*-BN. The interface between a (111) atomic plane of fcc Ni or fcc Co and a hexagonal basal plane of *h*-BN should be a near ideal spin filter for *p*-type *h*-BN but not for *n*-type *h*-BN. In each case, minority spin band electrons are predicted to be transmitted by the filter.

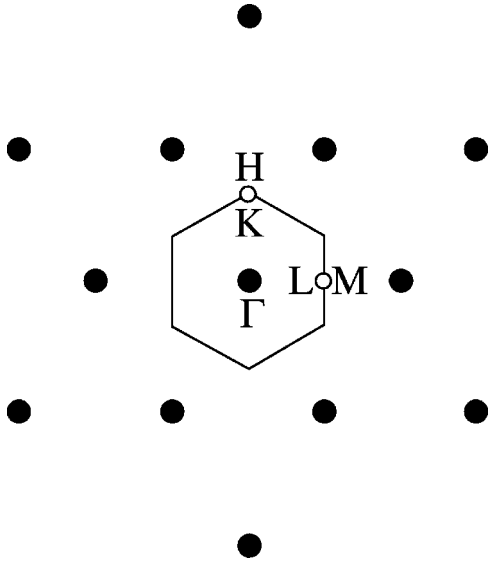

FIG. 2. Solid circles represent projections onto a hexagonal *h*-BN basal plane of the reciprocal lattice vectors of hcp and fcc Bravais lattices perfectly lattice matched to the *h*-BN basal plane and also the projections of the reciprocal lattice vectors of the *h*-BN onto that plane. The hexagon is the projections of the first Brillouin zone of the hcp lattice and of *h*-BN onto the same plane; Open circles indicate the projections of the *H*, *K*, *L*, and *M* points on the Brillouin zone boundary onto the plane.

3. Boron nitride with the zinc blende and wurtzite crystal structures

While *h*-BN is the stable form of boron nitride under normal conditions, BN can also exist with the zinc blende and wurtzite crystal structures, and band structure calculations have been performed for those systems as well.[39] Both are indirect gap materials with the valence band maximum at Γ. The conduction band minima are at *X* for the zinc blende form and at *K* for the wurtzite.[39] The hexagonal atomic planes of these materials should lattice match reasonably well to the hexagonal atomic planes of hcp Co, fcc Ni, and fcc Co.

The present theory makes the following predictions for these interfaces based on the Co and Ni band structures in Refs. 27–29: The interfaces between the hcp Co and both the zinc blende and wurtzite BN semiconductors should be near-ideal spin filters for both *p*-type and *n*-type semiconductors. This should also be true of interfaces between the fcc Ni and Co and the wurtzite form of BN. However, the interfaces between the fcc Ni and Co and the zinc blende form of BN should be near-ideal spin filters for the *p*-type BN but not for the *n*-type BN. In the case of fcc Co with *p*-type BN having the zinc blende or wurtzite structures see also Ref. 30.

4. Strained germanium (111) films

Another indirect gap semiconductor that meets the criteria for a near-ideal spin filter is (*n*-type or *p*-type) Ge in the form of a thin, highly strained film whose (111) face is in

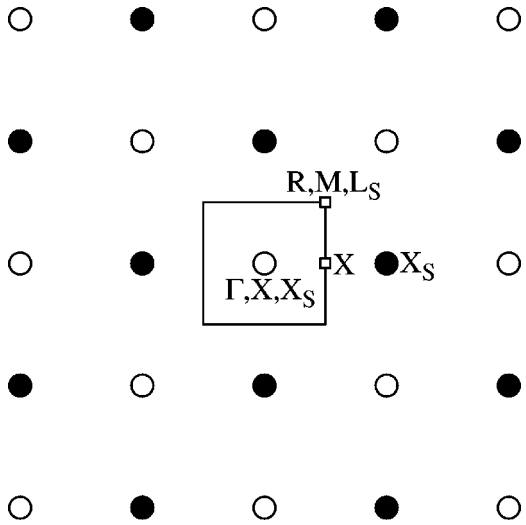

FIG. 3. Open circles represent projections onto the interface plane of the reciprocal lattice vectors of a semiconductor with the zinc blende or diamond structure perfectly lattice matched at a (001) interface to CoS_2. Open and solid circles represent projections of the reciprocal lattice vectors of CoS_2 onto the interface plane. The square is the projection of the first Brillouin of CoS_2 onto the same plane. X_S and L_S denote projections of some X and L points of the semiconductor Brillouin zone onto the interface plane. X, R, and M denote projections of the respective points of the CoS_2 Brillouin zone onto the interface plane.

atomic registry with a (001) face of hcp Co or a (111) face of fcc Ni or Co. In this case the tensile in-plane strain experienced by the Ge would lift the degeneracy between its conduction band minima and the lowest conduction band minimum (at L in the [111] direction) would satisfy the wave vector selection rule criteria in Sec. II, as would the valence band maximum at the zone center.[30]

C. Spin filters involving the ferromagnet CoS_2

The above examples of spin filters all involve hcp Co, fcc Ni, or fcc Co as the ferromagnetic metal. Another ferromagnetic metal that will be shown below to be an interesting candidate for spin filters is CoS_2 which has a simple cubic Bravais lattice with a lattice parameter $a=5.407$ Å. The lattice parameters of several semiconductors with the zinc blende and diamond crystal structures have values very close to this, so that accurate lattice matching at interfaces between (001) crystal planes of those semiconductors and a (001) plane of CoS_2 is possible. Figure 3 shows the projections onto a (001) interface plane of the reciprocal lattice vectors of CoS_2 (open and solid circles) and of a semiconductor with the zinc blende or diamond crystal structure (open circles) exactly lattice matched to the CoS_2 at the interface. The square is the projection of the first Brillouin zone of CoS_2. X_S and L_S denote projections of some X and L points of the semiconductor Brillouin zone onto the interface plane. X, R, and M denote projections of the respective points of the CoS_2 Brillouin zone onto the interface plane. Band structure calculations[32] indicate that the projection of the majority electron Fermi surface of CoS_2 onto the (001) plane occupies most of the projection of the first Brillouin zone onto the (001) plane but not the immediate vicinity of the corners, whereas the projection of the minority Fermi surface forms diagonal cross-shaped regions centered on the corner points R. Thus for a semiconductor whose Fermi surface is at the center of the Brillouin zone or at or near the zone boundary point X, according to the criteria in Sec. II, only majority spin band electrons are transmitted at the Fermi energy from CoS_2 into the semiconductor through the lattice matched (001) interface, while for a semiconductor whose Fermi surface is at or near the zone boundary point L, only minority spin band electrons are transmitted at the Fermi energy from CoS_2 into the semiconductor through the lattice matched (001) interface. Thus most semiconductors with the zinc blende or diamond structures whose lattice parameters match CoS_2 at a (001) interface should be considered candidates for spin filters with CoS_2.

Some examples of semiconductors with the zinc blende and diamond structures that approximately lattice match CoS_2 in the above sense [and thus are candidates for spin filters with CoS_2 and a (001) interface] are listed below. The name of the semiconductor is followed in parentheses by the ratio a_p/a of the value a_p of the lattice parameter required for a perfect match to CoS_2, to the actual value a of the lattice parameter for the semiconductor: CuCl(1.000), ZnS(0.999), Si(0.996), GaP(0.993), AlP(0.989), AlAs(0.959), Ge(0.956), GaAs(0.956), ZnSe(0.954), CuBr(0.950), CdS(0.928), and InP(0.921).

Note that the technologically important semiconductor Si is a very good lattice match for CoS_2, and that the matching may be improved further by alloying the Si with a small amount of C or working with thin films and a slightly strained interface.

D. Spin filters involving FeAl, τ-MnAl, Pd_3Fe, or Co_3Pt

Their calculated band structures[33,34] indicate that both FeAl and τ-MnAl do not satisfy Eq. (7) for some combinations of interface orientation and spin, a necessary but not sufficient condition for a ferromagnetic metal to be an ideal spin filter in conjunction with a semiconductor whose Fermi surface is close to the center of the Brillouin zone. FeAl is a cubic material and does not satisfy Eq. (7) for the majority spin Fermi surface and (110) interfaces. Its lattice parameter is close to one-half of those of several semiconductors with zinc blende or diamond crystal structures so that a good lattice match between FeAl and those semiconductors at a (110) interface is possible. τ-MnAl has a tetragonal structure. Its lattice parameter in the plane with fourfold symmetry is also close to one half of those of some semiconductors with zinc blende and diamond crystal structures, so that a good lattice match with (001) faces of those semiconductors is possible. The minority spin Fermi surface of τ-MnAl does not satisfy Eq. (7) for these interfaces. But a detailed analysis of these systems, taking account of nonzero reciprocal lattice vectors in Eqs. (6) and (8), shows that they do not satisfy the criteria for ideal spin filters for semiconductors whose Fermi surfaces are close to the center of the Brillouin zone or to X. The published Fermi surface data[33,34] are not complete

enough to decide whether these systems should be near-ideal spin filters with semiconductors whose Fermi surfaces are near L. However, for strained thin films of n-type semiconductors with zinc blende or diamond structures and Fermi surfaces near X in the Brillouin zone and in atomic registry with τ-MnAl at a (001) interface as above, if the interfacial strain is such that it lowers the conduction band minima at $(\pm k,0,0)$ and $(0,\pm k,0)$ relative to those at $(0,0,\pm k)$ sufficiently that the conduction band minima at $(0,0,\pm k)$ are emptied of electrons, then the (001) interface is predicted to be an ideal spin filter at low temperatures and bias voltages. This is because the majority spin Fermi surface of τ-MnAl intersects the line RX at the edge of the Brillouin zone while the minority spin Fermi surface does not.[34]

Pd_3Fe is a ferromagnetic metal with the Cu_3Au crystal structure and a simple cubic Bravais lattice. The calculated band structure of this material[41] satisfies Eq. (7) for both the majority and minority spin Fermi surfaces. Therefore Pd_3Fe does not satisfy the criteria for ideal spin filters with semiconductors whose Fermi surfaces are near the center of the Brillouin zone. However, the size of the lattice parameter of Pd_3Fe is close to a factor of $\sqrt{2}$ smaller than those of some semiconductors with the zinc blende and diamond crystal structures, making an approximate lattice match at a (001) interface possible with a 45° relative rotation of the Bravais lattices about the (001) axis. For strained thin films of such n-type semiconductors with conduction band minima at X in atomic registry with Pd_3Fe, the (001) interface is again predicted to be an ideal spin filter at low temperatures and bias voltages provided that the interfacial strain shifts the conduction band minima in the same way as is described above for τ-MnAl systems. This is because the spin down Fermi surface of Pd_3Fe intersects the line RM at the edge of the Brillouin zone while the spin up Fermi surface does not.[41]

According to recent band structure calculations,[42] Eq. (7) is satisfied for both the majority and minority spin Fermi surfaces of Co_3Pt; the majority spin Fermi surface intersects the line MX at the edge of the Brillouin zone while the minority spin Fermi surface does not, and the line RM intersects both Fermi surfaces. Based on this, (001) interfaces (similar to those described above for Pd_3Fe), with atomic registry between Co_3Pt and semiconductors with the zinc blende and diamond crystal structures, are predicted to be ideal spin filters for semiconductors whose Fermi surfaces are close to L but not for semiconductors whose Fermi surfaces are close to X or close to the center of the first Brillouin zone.

E. Spin filters involving Gd or Tb

Gd and Tb are ferromagnetic metals with the hcp structure. Their lattice parameters in the (001) basal plane with hexagonal symmetry are 3.6336 and 3.6055 Å, respectively, an approximate match to the hexagonal planes of several semiconductors with the zinc blende, diamond, and wurtzite structures. The Fermi surfaces of Gd and Tb are still not completely understood; the present analysis is based on the Fermi surface calculations of Ahuja *et al.*[35] These calculations suggest that for Gd and Tb and (001) interface planes Eq. (7) is satisfied neither on the minority spin Fermi surface nor on the majority spin Fermi surface, and that only the Fermi surface for the majority spin electrons is present at high symmetry lines HK, KM, and LM on the Brillouin zone boundary. Based on this, semiconductors lattice matched as above and having Fermi surfaces that project onto the interface plane near the edges of the projection of the Brillouin zone of Gd and Tb should be candidates for near ideal spin filters with Gd and Tb. Some examples are Si(0.946,0.939), AlP(0.940,0.933), GaP(0.943,0.936), and BAs(1.076,1.067) where the numbers in parentheses indicate the accuracy of the match for Gd and Tb, respectively. The accuracy of the matching is only fair but may be improved in strained epitaxial thin films or by semiconductor alloying.

F. Spin filters involving magnetic superlattices

Ferreira *et al.* have recently suggested that a pair of magnetic superlattices connected by a conducting medium with a low carrier density should function as a perfect spin filter[22] if Eq. (7) is satisfied on the majority spin Fermi surface of the superlattice but not on the minority spin Fermi surface or vice versa. However, they did not identify a material that may serve as their conducting medium with a low carrier density.

In this section, I examine the possibility that the interfaces between some ferromagnetic superlattices and semiconductors may be ideal spin filters for transmission of spin-polarized electrons from the superlattice to the semiconductor, and also the possibility that semiconductors may be suitable conducting media with low carrier densities for devices of the type proposed by Ferreira *et al.* In both cases it turns out to be necessary to go beyond consideration of Eq. (7) and I base the analysis on the theory of Sec. II.

The calculated minority spin Fermi surface of the (100)-oriented superlattice Fe_4/Cr_4 (Ref. 36) satisfies Eq. (7) for (100) interfaces while the majority spin Fermi surface does not. The superlattice has a lattice parameter in the (100) plane that is very close to one-half of those of GaAs, AlAs, Ge, ZnSe, and CuBr, so that very good atomic registry between Fe_4/Cr_4 and these semiconductors at a (001) interface is possible. The analysis of these interfaces as candidates for nearly ideal spin filters in terms of the criteria of Sec. II is as follows: The projection onto the interface plane of a reciprocal lattice vector of the semiconductor Bravais lattice connects the projection of the center of the Brillouin zone of the Fe_4/Cr_4 superlattice to the projection of the corner of the Brillouin zone. Assuming that the electronic structure of the superlattice is as in Ref. 36, this implies that the transmission of neither majority nor minority spin electrons is forbidden from this superlattice to semiconductors (lattice matched to the superlattice as above) whose Fermi surfaces are near the center of the Brillouin zone or near X. Furthermore, the projection of neither the majority nor the minority spin Fermi surface of the superlattice is connected by the projection of a reciprocal lattice vector to the projection of a semiconductor Fermi surface located at L. Thus despite the (100) Fe_4/Cr_4 superlattice satisfying Eq. (7) for one spin species and not for the other, its calculated electronic structure[36] indicates that it

is not suitable for use in spin filters with semiconductors lattice matched in this way, except possibly for strained thin semiconductor films with Fermi surfaces near *X*, as has been described above for τ-MnAl. The same applies to the use of such semiconductors as the conducting medium with low carrier density in devices of the type proposed by Ferreira *et al.* with the (100) Fe_4/Cr_4 superlattice.

Some other magnetic superlattices whose calculated electronic structures[31] satisfy Eq. (7) on their spin down Fermi surfaces but not on their spin up Fermi surfaces are Ni_nCo_m multilayers grown along the (111) direction. Spin filtering by interfaces between these superlattices and various semiconductors can be analyzed using the results of Sec. II [consideration of Eq. (7) alone is again insufficient] in a similar way to the interfaces of those semiconductors with Ni and Co that are treated in Sec. III B, with similar results. Thus such superlattices should, like Co and Ni crystals, be suitable for injecting spin polarized electrons into the same semiconductors. Devices of the kind proposed by Ferreira *et al.* based on these superlattices and semiconductors should also in principle be possible.

IV. DISORDER AT THE INTERFACE

The preceding sections have addressed ordered interfaces between ferromagnetic metals and semiconductors. Here I will consider the effects of disorder at the interface on spin filters (focussing particularly on intermixing disorder) by solving a simple tight-binding model numerically. For a perfectly ordered interface and a partly spin-polarized ferromagnetic metal, the model exhibits a regime in which the electron transmission through the interface is completely spin polarized; i.e., the interface is a perfect spin filter. On the other hand, for strong intermixing between the metal and semiconductor at the interface, a regime occurs in which the spin polarization of the electrons transmitted into the semiconductor is much less than the spin polarization of the electrons at the Fermi level in the ferromagnetic metal. I.e., mixing disorder at the interface can make the interface a spin ''antifilter'' by strongly spin *depolarizing* the electric current transmitted from the ferromagnet to the semiconductor, even in the absence of spin-flip scattering. This effect has a different origin from that described by Schmidt *et al.*[14] but should work in concert with the latter.

A. Model

The geometry of the model to be considered is shown in Fig. 4(a): Semi-infinite crystals of ferromagnet and semiconductor meet at a plane interface *d* layers thick where mixing between the ferromagnet and semiconductor occurs. It is assumed that in each of these *d* layers the semiconductor and ferromagnetic species are randomly distributed and that the average concentration of each species varies linearly with position through the interface. The model electronic Hamiltonian is

$$H=\sum_{i,\sigma}\epsilon_{i\sigma}a^{\dagger}_{i\sigma}a_{i\sigma}-\sum_{i,j,\sigma}t_{ij}a^{\dagger}_{i\sigma}a_{j\sigma}, \tag{9}$$

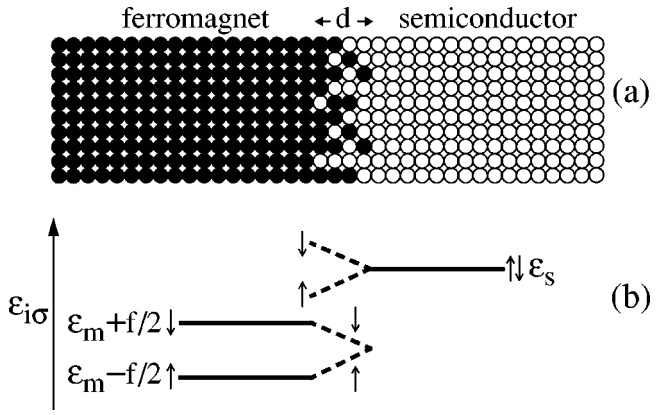

FIG. 4. (a) Schematic of semi-infinite ferromagnetic metal and semiconductor quantum wires that join at a disordered Ohmic interface *d* layers thick. (b) Tight-binding model site energies $\epsilon_{i\sigma}$ for majority $\uparrow$ and minority $\downarrow$ spin electrons in the ferromagnet and semiconductor (solid lines) and in the mixed region (dashed lines) that are shown above in (a).

where $a^{\dagger}_{i\sigma}$ creates an electron with spin σ on site *i* of the (simple cubic) lattice and t_{ij} is the hopping matrix element between sites *i* and *j*. The form of site energy $\epsilon_{i\sigma}$ is illustrated in Fig. 4(b): In the semiconductor region it is a constant independent of the spin $\epsilon_{i\sigma}=\epsilon_s$. In the ferromagnet it takes values $\epsilon_{i\sigma}=\epsilon_m\pm f/2$ where *f* is the energy splitting between minority and majority spin electron bands. It is assumed that in the interface region where the ferromagnetic and semiconductor species mix the site energies for the minority and majority spin electrons are given by the mean-field form $\epsilon_{i\sigma}=\epsilon_s\pm\alpha f/2$ or $\epsilon_{i\sigma}=\epsilon_m\pm\alpha f/2$ if the site is occupied by the semiconductor or ferromagnetic species, respectively; α is the average concentration of the ferromagnetic species in the interface layer in which $\epsilon_{i\sigma}$ is evaluated. The physical meaning of this assumption is that the electron-electron interaction effects that give rise to the energy splitting between the majority and minority spin electrons have a range of at least a few lattice sites and in the mixing region affect electrons on sites occupied by the semiconductor species as well as those occupied by the ferromagnetic species. The hopping matrix elements are assumed to be nearest neighbor and of the form $t_{ij}=t_s$ if *i* and *j* are both semiconductor sites, $t_{ij}=t_m$ if *i* and *j* are both ferromagnetic sites, and $t_{ij}=(t_s+t_m)/2$ if one of the sites is ferromagnetic and the other semiconductor.

B. Theoretical considerations and method of solution

According to the Landauer theory of transport[43] the electrical conductance *G* of a structure such as that in Fig. 4(a) is given by $G=e^2/h\Sigma_{kl\sigma}T^{\sigma}_{kl}$ where T^{σ}_{kl} is the probability that an electron with spin σ incident from the source (ferromagnet) in channel *l* at the Fermi energy is transmitted into channel *k* of the drain (semiconductor). Thus the spin-dependent Landauer transmission probabilities $T^{\sigma}=\Sigma_{kl}T^{\sigma}_{kl}$ are the appropriate measure of how well spin up and down electrons are transmitted through the interface and are studied in the present work. The results for T^{σ} presented here have been obtained by solving the Lippmann-Schwinger equation

$$\Psi_l^\sigma = \Phi_l^\sigma + G_0(E+i\epsilon)V\Psi_l^\sigma, \tag{10}$$

where $G_0(z)=(z-H_0)^{-1}$ and H_0 are the Green's function and Hamiltonian for the system shown in Fig. 4(a) but with no disorder present and with the ferromagnet decoupled from the semiconductor. I.e., H_0 is defined similarly to the Hamiltonian H given by Eq. (9) but with the width d of the intermixing region equal to zero and with $t_{ij}=0$ if one of the sites i,j is in the ferromagnet and the other in the semiconductor. $V\equiv H-H_0$ then contains the coupling between the ferromagnet and the semiconductor and any disorder that is present in the system. In Eq. (10), Φ_l^σ is the eigenstate of H_0 that corresponds to an electron with energy E and spin σ that travels from left to right in channel l of the (semi-infinite) ferromagnet and is reflected at the interface where the coupling to the semiconductor has been switched off ($t_{ij}=0$) in H_0. Here Ψ_l^σ is the corresponding eigenstate of the complete Hamiltonian H that is partly reflected at the interface and partly transmitted into the semiconductor. G_0 and Φ_l^σ were evaluated analytically. Ψ_j^σ was then evaluated by solving Eq. (10) numerically using matrix techniques. In the semiconductor region Ψ_j^σ was expressed in terms of its partial transmission amplitudes τ_{kl}^σ into the various semiconductor channels k. The partial transmission probabilities $T_{kl}^\sigma = |\tau_{kl}^\sigma|^2 v_k^\sigma / v_l^\sigma$ that enter T^σ were obtained using the calculated propagation velocities v_k^σ and v_l^σ of electrons at the Fermi energy with spin σ in channels k and l of the semiconductor and ferromagnet, respectively.

C. Results

Representative results are shown in Fig. 5. Here the metal and semiconductor regions of Fig. 4(a) are semi-infinite nanowires with a cross section of 15×15 lattice sites. $\epsilon_m = 0$ and $t_m > 0$. The exchange splitting between the majority and minority spin bands in the ferromagnet is 3 times the electron hopping parameter in the ferromagnet, $f=3t_m$. The semiconductor conduction bandwidth is half of the bandwidth of the metal, $t_s = t_m/2$. The Fermi energy E_F is in units of t_m. It should be noted that the essential qualitative properties of the results to be presented below are insensitive to the model parameters such as the cross section of the wire, the size of the exchange splitting f, and the relative sizes of the bandwidth parameters t_s and t_m in the ferromagnet and semiconductor and the conclusions drawn (other than those regarding mesoscopic fluctuations) will also apply to metal-semiconductor interfaces with areas that are macroscopic in size.

The overlapping majority and minority spin bands of the ferromagnet can be seen in Fig. 5(a) which shows the number n_m^σ of majority spin (solid line) and minority spin (dotted line) Landauer channels in the ferromagnet at the Fermi energy E_F as a function of E_F.

Figure 5(b) shows the calculated Landauer transmission probabilities T^σ for majority (solid line) and minority (dotted line) spin electrons from the ferromagnet to the semiconductor as a function of the Fermi energy, for a perfectly clean, sharp interface with no intermixing of the metal and semiconductor [$d=0$ in Fig. 4(a)]. For each value of E_F, the value of the site energy ϵ_s in the semiconductor has been chosen so that the electron density in the semiconductor conduction band (and the number n_s^σ of conducting channels at E_F in the semiconductor for each spin σ) is small relative to typical values for the metal; the results shown are for $n_s^\sigma = 6$.

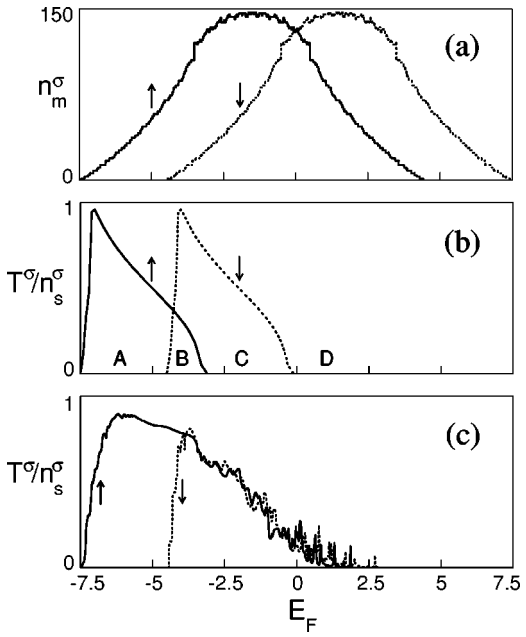

FIG. 5. Number of Landauer channels n_m^σ in the ferromagnetic quantum wire at the Fermi energy E_F (a) and calculated transmission probability T^σ from the ferromagnet to the semiconductor through a perfect (b) and disordered (c) interface for majority (solid lines) and minority (dotted) spin electrons at E_F vs E_F for the infinite quantum wire shown in Fig. 4(a).

In region A of Fig. 5(b) ($-7.5t_m < E_F < -4.5t_m$) only majority spin electrons are transmitted into the semiconductor because only they are present in the ferromagnet. In region B ($-4.5t_m < E_F < -3.1t_m$) both majority and minority spin electrons are transmitted into the semiconductor. In region C ($-3.1t_m < E_F < -0.1t_m$) *although both majority and minority spin electrons are present in the ferromagnet at the Fermi energy, only minority spin electrons are transmitted into the semiconductor*: The majority spin electrons are reflected perfectly at the metal-semiconductor interface and the system is an ideal spin filter—electron injection into the semiconductor is 100% minority spin polarized. In region D ($E_F > -0.1t_m$) both the majority and minority spin electrons are reflected perfectly at the interface and neither species is transmitted into the semiconductor.

The 100% spin polarization of the electrons transmitted into the semiconductor in region C is clearly not due to the difference between the majority and minority spin densities of states in the ferromagnet since the number of majority spin channels at the Fermi energy *exceeds* [see Fig. 5(a)] that of the minority spin channels throughout this energy range in which only the minority spin carriers are transmitted into the semiconductor. It is due instead to the selection rule associated with conservation of the component of the electron

wave vector parallel to the interface between the ferromagnet and semiconductor[44] and to the general property of semiconductors that under near-equilibrium conditions the conduction band electrons are confined to *very small* regions of k space near the conduction band minima: In this model the electron eigenenergies in the ferromagnet are $E^{\sigma}_{\mathbf{k}}=\epsilon_m - 2t_m[\cos(k_x a)+\cos(k_y a)+\cos(k_z a)]\pm f/2$ where a is the lattice parameter. The Fermi energy is close to the semiconductor conduction band minimum which in the present model is at $\mathbf{k}=\mathbf{0}$. With the interface perpendicular to the z axis, conservation of the components of the wave vector parallel to the interface requires that only electrons with k_x and k_y close to zero can be transmitted into the semiconductor at the Fermi energy. For $k_x=k_y=0$, $E^{\sigma}_{\mathbf{k}}=\epsilon_m-2t_m[2+\cos(k_z a)] \pm f/2$ which implies that $E^{\sigma}_{\mathbf{k}}\leqslant\epsilon_m-2t_m\pm f/2$. This means that only electrons with energies less than $\epsilon_m-2t_m\pm f/2$ can be transmitted from the ferromagnet to states at the bottom of the semiconductor conduction band. For the model parameters $\epsilon_m=0$ and $f=3t_m$ chosen in Fig. 5, this implies that majority and minority spin electrons can be transmitted from the ferromagnet to states at the bottom of the semiconductor conduction band at energies below $-3.5t_m$ and $-0.5t_m$, respectively. The corresponding high-energy cutoffs for transmission of majority and minority carriers in Fig. 5(b) are slightly higher, at $-3.1t_m$ and $-0.1t_m$, respectively, because in the numerical calculations the Fermi energy was chosen slightly above the semiconductor's conduction band minimum instead of right at the minimum as in the above analysis.

The calculated transmission probabilities of majority (solid line) and minority (dotted line) spin electrons from the ferromagnet to the semiconductor through a disordered interface are shown in Fig. 5(c). The model parameters are the same as in Fig. 5(b) except that now the thickness of the interface where mixing of the semiconductor and metal occurs is $d=8$ lattice layers. Since the physics of electron transmission through the perfect interface [Fig. 5(b)] is controlled by a selection rule associated with lattice periodicity parallel to the interface, one should expect the strongly disordered interface to behave differently; the differences between Figs. 5(b) and 5(c) are indeed striking: Whereas for the perfect interface transmission from the ferromagnet to the semiconductor is partly spin polarized in region B and completely spin polarized in region C of Fig. 5(b), the transmission is close to being completely spin unpolarized in the corresponding energy ranges for the disordered interface, as can be seen in Fig. 5(c). Here the interface acts as a spin ''antifilter'' with the spin polarization of the transmitted current being much less than even that of the electronic channels incident on the interface from ferromagnet. The differences between the total Landauer transmission probabilities of the majority and minority spin electrons through the disordered interface in this regime are governed by (pseudorandom) fluctuations of the transmission probabilities. Such quantum conductance fluctuations with an amplitude of order e^2/h that occur as the Fermi energy is varied are well known in other systems[45] and are the mesoscopic ''fingerprint'' of the specific microscopic configuration of the atoms in the disordered region. In energy region D these fluctuations are replaced by weak isolated quantum transmission resonances and whether majority or minority spin electrons or both are transmitted from the semiconductor into the ferromagnet at a particular energy is controlled by the microscopic details of the disorder in the interface.

Thus the intermixing at the interface between a ferromagnetic metal and semiconductor may act to strongly suppress the spin polarization of the transmitted current. In the present model, this suppression is found to be insensitive to the choice of the model parameters: Even if there are only $d=2$ disordered layers present at the interface, the spin polarization of the electron transmission in region C of Fig. 5 is reduced to $\sim 30\%$. Based on the considerations of Schmidt *et al.*[14] it may be difficult to detect a spin polarization of the electric current in this case in spin-valve resistance measurements on devices in which the transport through the semiconductor is diffusive.

V. SUMMARY AND SOME FURTHER CONSIDERATIONS

In this article it has been pointed out that certain atomically ordered interfaces between some ferromagnetic metals and semiconductors should act as ideal spin filters that transmit only electrons belonging to the majority spin bands of the ferromagnet or only electrons belonging to the minority spin bands at the Fermi energy. Criteria for determining which combinations of ferromagnetic metal, semiconductor, and interface should have this property have been formulated, and examples of systems that meet these criteria to a high degree of precision have been described.

The criteria depend only on the bulk band structures of the semiconductor and ferromagnetic metal and on the translational symmetries of the semiconductor, metal, and interface. Thus they do not depend on whether a Schottky barrier is present at the interface or on the strength of this barrier. If there is a strong Schottky barrier, then although the interface may obey the criteria and be an ideal spin filter at low and moderate bias, the current that it transmits will be weak. The size of the Schottky barrier depends on the materials involved, and it is reasonable to expect that among the many systems that should be nearly ideal spin filters some will have low Schottky barriers.

Estimates of the Schottky barrier heights for some of the systems of interest may be obtained using the model of Tersoff[46] which expresses the Schottky barrier height in terms of semiconductor band gap parameters and a phenomenological fitting term δ_m that depends only on the metal m. A reasonable value for this parameter for Co and Ni is $\delta_{Co}=\delta_{Ni}=-0.2$ eV which yields Schottky barrier height estimates of 1.2, 0.6, 0.0, -0.3, and 1.2 eV for interfaces between n-type ZnTe, GaSb, InAs, CdSe, and CuI, respectively, and Ni or Co. These estimates suggest that the spin-filter interfaces between n-type InAs or CdSe and Ni or Co may be Ohmic for the transmitted spin species. However, their reliability is uncertain. For example, δ_{Au} has been estimated to be also -0.2 eV.[46] Based on this, within the Tersoff model, the Schottky barrier heights for Ni and Co should be close to those for Au, but the Schottky barrier height for Au on n-type CdSe has been measured to be 0.49 eV.[47]

A method commonly used to reduce Schottky barriers is to interdiffuse the metal and semiconductor. This, however, breaks the translational symmetries of the interface and should therefore degrade its spin filtering property. As has been shown in Sec. IV, such intermixed interfaces can have spin antifiltering properties, with the transmitted electrons being much less spin polarized than even those in the ferromagnetic metal at the Fermi energy. This in concert with the mechanism of Schmidt *et al.*[14] may help to account for some of the setbacks that have been encountered in experimental attempts to inject strongly spin-polarized electrons from ferromagnetic metals into semiconductors. A potentially better way to reduce Schottky barriers in candidates for ideal spin filters is to modify the chemistry of the interface by introducing a suitable adsorbate between the metal and semiconductor during growth. Ohmic contacts between Al and InGaAs(001) have been made in this way by introducing a Si bilayer between the Al and InGaAs.[48] If the adsorbate is atomically ordered and its presence does not change the translational symmetries of the system parallel to the plane of the interface, then the system with the adsorbate will still conform to the criteria for an ideal spin filter if the system without the adsorbate does. Thus this is a promising method for manipulating Schottky barriers while preserving the spin filtering property of the interface. Inserting a suitable atomically ordered intermediate layer between the semiconductor and ferromagnetic metal may also help to enhance the degree of atomic order at the interface while preserving its spin filtering property: Since an ordered commensurate monolayer of *h*-BN is known to grow well on (111) surfaces of fcc Ni,[37] introducing one or more monolayers of *h*-BN at the interface between the semiconductors and metals in Sec. III B is an interesting possibility in this regard. A more standard method for suppressing Schottky barriers is to heavily dope the semiconductor. Since the concentration of dopant atoms in heavily doped semiconductors is still much smaller than that of the intrinsic semiconductor species, it is reasonable to expect the spin filtering property of an interface not to be degraded greatly by this method of Schottky barrier suppression, making it a better choice than interdiffusion of the ferromagnetic metal and semiconductor.

While the criteria for ideal spin filters guarantee that only electrons from the majority spin bands of the ferromagnet or only those from the minority spin bands are transmitted into the semiconductor at the Fermi energy, the degree of spin polarization of the electrons injected into the semiconductor can be influenced by spin-flip scattering if that occurs at the interface. Spin-orbit coupling can also result in the electron states of the majority and minority spin bands of the ferromagnet being incompletely spin polarized. The nominally spin up electron eigenstates of semiconductor may also contain an admixture of spin down (and vice versa), due to spin-orbit coupling. Since the linear combinations of spin up and spin down in the eigenstates of the ferromagnet and semiconductor need not in general match, spin-orbit coupling can limit the degree of spin polarization of the carriers injected into the semiconductor. Thus it is desirable to choose materials in which spin-orbit coupling of the relevant states is minimal, either because of the low atomic numbers of the constituent elements (as in the semiconductors BN and Si) or because of the material's band structure.

ACKNOWLEDGMENTS

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