Boltzmann theory of engineered anisotropic magnetoresistance in (Ga,Mn)As

T. Jungwirth1,2, M. Abolfath3, Jairo Sinova2, J. Kučera1, and A.H. MacDonald2
1Institute of Physics ASCR, Cukrovarnická 10, 162 53 Praha 6, Czech Republic
2Department of Physics, The University of Texas at Austin, Austin, TX 78712
3Department of Physics and Astronomy, University of Oklahoma, Norman, OK 73019-0225
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We report on a theoretical study of dc transport coefficients in (Ga,Mn)As diluted magnetic semiconductor ferromagnets that accounts for quasiparticle scattering from ionized Mn$^{2+}$ acceptors with a local moment $S = 5/2$ and from non-magnetic compensating defects. In metallic samples Boltzmann transport theory with Golden rule scattering rates accounts for the principle trends of the measured difference between resistances for magnetizations parallel and perpendicular to the current. We predict that the sign and magnitude of the anisotropic magnetoresistance can be changed by strain engineering or by altering chemical composition.

In most (III,V) semiconductors, Mn$^{2+}$ substitution on a cation (column III element) site introduces an $S = 5/2$ local moment and a valence band hole $\mathbb{1}$. Mn$_{III_{1-x}}$V diluted magnetic semiconductors (DMSs) are ferromagnetic and metallic for Mn fractions larger than $x \sim 1\%$. Many magnetic properties of the most robust ferromagnetic samples, those that have $\sim 5\%$ or more Mn and are annealed to reduce the density of compensating defects, appear to be adequately explained by virtual crystal approximation models in which disorder is ignored $\mathbb{1}$. For example in bulk DMSs, this approach can account for ferromagnetic critical temperatures $\sim 100$ K $\mathbb{1}$, the correlation between magneto-crystalline anisotropy and substrate lattice constant $\mathbb{2}$, the size and sign of the anomalous Hall effect $\mathbb{1}$, and several optical properties $\mathbb{3}$. It has also been used to describe properties of DMS heterostructures $\mathbb{4}$, $\mathbb{5}$, $\mathbb{6}$, $\mathbb{7}$, $\mathbb{8}$. We find that transport properties of these metallic ferromagnets are particularly helpful.

In this letter we investigate theoretically the $T = 0$ dc transport coefficients of (Ga,Mn)As ferromagnetic semiconductors. We find that relaxation-time-approximation solutions of the Boltzmann equation provide anisotropic magnetoresistance (AMR) estimates that are in good agreement with experiments $\mathbb{9}$, $\mathbb{10}$. Our results suggests that transport properties of these metallic ferromagnets can be understood within a conventional framework in which disorder is treated as a weak perturbation. We find that the conductivity varies by several percent when the magnetic order parameter is reoriented by a weak magnetic field, and predict that the magnitude and sense of this change depends on the chemical composition and on the substrate on which the thin film DMS ferromagnet is epitaxially grown. This spontaneous magnetoresistance anisotropy is the transport analog of magneto-crystalline anisotropy $\mathbb{11}$ which has approximately the same size relative to the total condensation energy of the ordered state. All results presented in this paper are for the (Ga,Mn)As DMS's. A large database that details our predictions for the AMR of many other host semiconductors over a wide range of compositions and strains is available on the internet $\mathbb{12}$.

We consider a microscopic Hamiltonian in which valence band holes interact with randomly located spins of substitutional Mn$^{2+}$ impurities via exchange interactions, and with randomly located ionized defects and each other via Coulomb interactions. Focusing on $T = 0$, we assume that the Mn spins are fully aligned in the ferromagnetic ground state. In the virtual crystal approximation, the interactions are replaced by their spatial averages, so that the Coulomb interaction vanishes and hole quasiparticles interact with a spatially constant Zeeman field. The unperturbed Hamiltonian for the holes then reads $H_0 = H_L + J_{pd} N_{Mn^{2+}} \Omega \cdot \vec{s}$, where $H_L$ is the six-band Kohn-Luttinger Hamiltonian $\mathbb{3}$, $\Omega$ is the Mn local moment orientation, $J_{pd} = 55$ meV nm$^3$ $\mathbb{4}$ is the local-moment – valence-band-hole kinetic-exchange coupling constant, $N_{Mn^{2+}}$ is the density of ordered Mn local moments, and $\vec{s}$ is the envelope-function hole spin operator $\mathbb{5}$. We use the relaxation-time-approximation solution to the semiclassical Boltzmann equation to estimate the dc conductivity tensor:

$$
\sigma_{\alpha\beta} = \frac{e^2}{h} N \sum_{n,k} \left( \hbar \Gamma_{n,k} \right)^{-1} \frac{\partial E_{n,k}}{\partial k_{\alpha}} \frac{\partial E_{n,k}}{\partial k_{\beta}} \delta(E_F - E_{n,k}),
$$

where $\Gamma_{n,k}$ is the quasiparticle elastic scattering rate, $n$ and $k$ are the band and wavevector indices of the valence band Bloch states of the unperturbed system, and $E_{n,k}$ are the spin-split band energies of the ferromagnetic state. In Eq. (1) we have omitted the asymmetric terms in the off-diagonal elements of $\sigma_{\alpha\beta}$ that contribute to the anomalous Hall conductivity, discussed in detail elsewhere $\mathbb{11}$. The symmetric off-diagonal elements, described by Eq. (1), vanish when the magnetization is aligned along one of the cube edges of the host lattice.

In our model, itinerant holes are scattered on substitutional Mn$^{2+}$ impurities by a Thomas-Fermi screened Coulomb potential and by a magnetic-kinetic-exchange potential. For majority-spin holes both potentials are attractive while for minority-spin holes the magnetic potential becomes repulsive. We estimate the transport
weighted scattering rate from Mn$^{2+}$ impurities using Fermi’s golden rule:

$$\Gamma_{\text{Mn}^{2+}} = \frac{2\pi}{\hbar} N_{\text{Mn}^{2+}} \int_{n} \frac{d\tilde{k}^2}{(2\pi)^3} |M_{n,n'}^{\text{E,F}}|^2 \times \delta(E_{n,\tilde{k}} - E_{n',\tilde{k}})(1 - \cos \theta_{\text{E,F}}),$$

where the scattering matrix element was approximated by the following expression,

$$M_{n,n'}^{\text{E,F}} = J_{pd} S(z_n^k \hat{\Omega} \cdot \hat{s}_{n',\tilde{k}^*})$$

$$- \frac{e^2}{\epsilon_{\text{host}}(k - \tilde{k})^2 + q_{TF}^2} \langle z_n^k | z_{n',\tilde{k}^*} \rangle.$$  

Here $\epsilon_{\text{host}}$ is the host semiconductor dielectric constant, $|z_n^k\rangle$ is a six-component envelope-function eigenspinor of the Hamiltonian $H_0$, and the Thomas-Fermi screening wavevector was approximated by the parabolic band expression, $q_{TF} = \sqrt{3e^2/2(2\epsilon_{\text{host}}\epsilon_0E_F)}$, where $p$ is the itinerant hole density and $E_F$ is the Fermi energy.

Recent experiments have established that magnetic and transport properties of (III,Mn)V DMS ferromagnets are sensitive to post-growth annealing protocols, and that this sensitivity is associated with changes in the density of defects that compensate the Mn$^{2+}$ acceptors. Our model recognizes that the transport properties of these materials are not determined solely by the scattering from substitutional Mn$^{2+}$ impurities and allows explicitly for scattering from compensating defects. We assume that compensation can occur due to the presence of As-antisite defects (common in low-temperature MBE grown GaAs hosts) or due to Mn interstitials. As-antisite defects are non-magnetic and can also be modeled as scattering from compensation due to As-antisites alone (i.e. no Mn-interstitials present). The substrate – DMS lattice mismatch, $\epsilon_0 \equiv (a_{\text{sub}} - a_{\text{DMS}})/a_{\text{DMS}}$, is between -0.002 and -0.003 in this case [4,16]. (Note that $a_{\text{sub}}$ and $a_{\text{DMS}}$ are the lattice constants of a fully relaxed substrate and ferromagnetic layer, respectively.) The parameters of the six-band Kohn-Luttinger model and strain coefficients used in these calculations are given in [21]. We also show in Fig. 1b separate contributions from individual heavy- and light-hole bands and demonstrate that in the ferromagnetic state the current is carried mostly by the majority-spin heavy-holes, a property that will be important for understanding the spin-injection properties of (III,Mn)V DMS ferromagnets.

As mentioned above, strong spin-orbit coupling in the semiconductor valence band leads to a variety of magneto-anisotropy effects [22]. For dc transport the in-plane conductivity along, e.g. the $x$-direction should change when the magnetization is rotated by applying a magnetic field stronger than the sample’s magneto-crystalline anisotropy field. In Fig. 2 we show the anisotropic magnetoresistance coefficients, $AMR_{\text{ip}} \equiv | \rho_{xx}(\hat{\Omega}|x) - \rho_{xx}(\hat{\Omega}|y) | / \rho_{xx}(\hat{\Omega}|y)$ and $AMR_{\text{op}} \equiv | \rho_{xx}(\hat{\Omega}|x) - \rho_{xx}(\hat{\Omega}|z) | / \rho_{xx}(\hat{\Omega}|z)$, for orthogonal magnetization directions in the plane of the thin ferromagnetic layer, and for one of the magnetization directions along the growth direction, respectively. The Mn fraction assuming As-antisite compensation alone is indicated in the figure by $x_1$. The total Mn fraction (including substitutional Mn$^{2+}$ atoms and Mn-interstitial atoms) for compensation due to interstitial Mn alone is labeled by $x_2$. The plots demonstrate that in (Ga,Mn)As/GaAs ferromagnets, which have compressive strain ($\epsilon_0 < 0$), $AMR$ is negative for typical chemi-
cal compositions, and $|\text{AMR}_{\text{ip}}| < |\text{AMR}_{\text{op}}|$. (Note that $\text{AMR}_{\text{ip}} = \text{AMR}_{\text{op}}$ in unstrained cubic DMSs.) The main plot shows that for a fixed hole density ($p = 0.4 \, \text{nm}^{-3}$) the magnitude of the AMR decreases from $\sim 10\%$ to $\sim 1\%$ with increasing Mn fraction. All those observations are consistent with available experimental data on $(\text{Ga,Mn})\text{As}$ DMS’s [15,16]. A more detailed comparison to measurements by Gallagher et al. [16] shows that theoretical data assuming As-antisite compensation only overestimate the decrease of AMR with increasing Mn fraction. Better quantitative agreement is obtained for compensation from Mn-interstitials, which is consistent with the presumed dominance of Mn-interstitial defects over As-antisite defects in the samples measured by Gallagher et al. [10].

In addition to this AMR engineering through doping that has been confirmed experimentally, our theory predicts a large sensitivity of the spontaneous transport anisotropy to strain. While strain does not play a significant role for AMR$_{\text{ip}}$, as one might expect from symmetry considerations, AMR$_{\text{op}}$ can change by more than 10% over the range of strains that can be achieved in the thin ferromagnetic layers by a proper choice of the substrate [1]. For larger Mn concentrations, AMR$_{\text{op}}$ is predicted to become positive in samples with tensile strain, as shown in the main plot of Fig. 2.

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FIG. 2. Anisotropic magnetoresistance coefficients as a function of strain (main plot and lower inset) and hole density (upper inset). Mn fractions corresponding to compensation due to As-antisites alone and Mn-interstitials alone are labeled as $x_1$ and $x_2$ respectively.