Transport Spin polarization of high Curie temperature MnBi films

Pushkal Thapa¹
Boris Nadjgorn⁴

Parashu Kharel²,³
Pavel Lukashev²,³
Renat Sabirianov³,⁴
Evgeny Tsymbal²,³
David Sellmyer²,³

¹Department of Physics and Astronomy, Wayne State University, Detroit, Michigan 48201, USA
²Department of Physics and Astronomy, University of Nebraska, Lincoln, Nebraska 68588, USA
³Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, Nebraska 68588, USA
⁴Department of Physics and Astronomy, University of Nebraska, Omaha, NE, 68182, USA
Why MnBi?

Spin injection from ferromagnet to semiconductors needs well-conducting ferromagnet with high Curie temperature, and high spin polarization (~half metallic)

MnBi is a good candidate as spin injector due to its
- high Curie temperature (628K)
- resistivity being dependent on power law of T as for half metals (so that the interfacial resistance can be high enough, also the interface properties may be controlled by addition of Bi)
- high coercivity with rectangular hysteresis loop
- large perpendicular room temperature anisotropy in thin films
- stable ferromagnetic phase (in NiAs structure, at room temperature)
- potential to be half metallic (in Zinc blende structure, it is predicted half metallic but it is metastable phase and difficult to grow epitaxially).

Finding the relationship between Spin polarization and magnetization

Spin transport properties are important to know in stable NiAs structure. This helps even to understand MnBi junctions that show ~70% magnetoresistance at room temperature. (E. Clifford, M. Venkatesan, and J. M. D. Coey, J. Magn. Magn. Mater. 272–276, 1614 (2004).
Normal metal

Andreev reflection

A.F. Andreev, Sov. Phys. JETP 19, 1228 (1964)

For Half-Metals Andreev reflection is suppressed

Half metal

No state available
-eV

Metal (P=100%)
Point Contact Andreev Reflection (PCAR) technique

![Diagram of PCAR setup]

- **Nb tip**
- **Superconducting tip**
- **Sample**
- **V, G, A**

**Graph:**
- Normalized Conductance vs. \( \frac{V}{\Delta} \)
- Z = 0.55, P = 0
- Z = 0, P = 50%

**References:**

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The spin-polarized fraction $\lambda$ of the current can not Andreev-reflect and thus does not contribute to the overall conductance below the gap.
MnBi Samples

- Prepared by sequential evaporation of Mn and Bi by e-beam evaporation on glass substrate

- The atomic ratio was Mn:Bi = 55:45

- Annealed in situ.

- Four such samples were prepared (Samples A, B, C, D)

- Difficult to make high quality samples
X-ray-diffraction spectra for orientation of MnBi films

- single phase MnBi
- highly textured polycrystalline films
- small traces of Bi detected
- strong diffraction peaks from (002) and (004) planes show preferred c-axis orientation of the films.
- hexagonal NiAs crystal structure
Resistivity of MnBi films

-MnBi samples are metallic

-residual resistivity at 4K is ~15µΩcm

-residual resistivity ratio (rrr) of ~8.5

-For T< 30K, resistivities of the film show an unusual T$^3$ dependence, similar to the observation for half metals such as CrO$_2$.

-Inset: fit for $\rho \sim T^{2.9}$ for T<30K
Sample A

- 32 nm thick
- Deposited at room temperature
- Annealed in situ for 1 hr at 410 °C

\[ P_{Z=0} = 63 \pm 0.8\% \]

Sample B

- 47nm
- Deposited at 125 °C
- Annealed at 350 °C for 1.5hr

\[ R_c = 17.1 \, \Omega \]
\[ T = 1.4K \]
\[ \Delta = 1.5 \, \text{meV} \]
\[ Z = 0.305 \]
\[ P = 0.491 \]
\[ R_c = 50.5 \, \Omega \]
\[ T = 1.4K \]
\[ \Delta = 1.5 \, \text{meV} \]
\[ Z = 0.283 \]
\[ P = 0.52 \]

\[ P_{z=0} = 57.8 \pm 1.6\% \]
Sample C

- 32 nm thick
- Deposited at room temperature
- Annealed for 1 hour at 400 °C

\[ T = 1.5K \]
\[ \Delta = 1.5mV \]
\[ Z = 0.461 \]
\[ P = 0.486 \]

\[ R_c = 28.8 \Omega \]

\[ T = 1.9K \]
\[ \Delta = 1.5mV \]
\[ Z = 0.419 \]
\[ P = 0.529 \]

\[ R_c = 49.2 \Omega \]

\[ P_{z=0} = 54.2 \pm 2.4\% \]
Sample D

- 32nm
- Deposited at 125 °C
- Annealed at 350 °C for 1 hr

\[ T = 1.5K \]
\[ \Delta = 1.5 \text{ mV} \]
\[ Z = 0.413 \]
\[ P = 0.439 \]
\[ R_c = 39 \Omega \]

\[ P_{Z=0} = 51.7 \pm 1.1\% \]
Polarization (P) vs. Saturation magnetization for other materials

\[ \text{Ni}_{1-x}\text{Fe}_x \]

\( d \) electrons (localized) – magnetic moment

\( sp \) electrons (itinerant) – spin polarization

- P is composition independent but saturation magnetization is higher for more Fe concentration.
- No correlation between the spin polarization and magnetic moment in \( \text{Ni}_x\text{Fe}_{1-x} \)

Nadgorny et. al., PRB Rapid Com 61, (2000)


\( \triangleright \) TSP at 0.25 K (□, Δ and +) and magnetization (●) at 5 K as a function of the V and Pt atomic fractions.

\( \triangleright \) The TSP (for \( \text{Al}_2\text{O}_3 \)) is proportional to the corresponding magnetization of the Co-V or Co-Pt alloy in the inset.

Kaiser et. al., PRL 94, 247203 (2005)
Magnetization and spin polarization

- MnBi thin films are anisotropic, Magnetization easy axis is perpendicular to the sample plane.
- Magnetization and coercivity depend on sample preparation condition.

Spin polarization is proportional to saturation magnetization.
Different degree of structural disorder in our samples may be the cause of variation of saturation magnetization.

Fixed Spin Moment method
Linear relation between $P_T$ and moment is the consequence of nearly linear variation of exchange splitting of the spin bands with the magnetic moment.

Ballistic, $\lambda \gg d$

Diffusive, $\lambda \ll d$

Ballistic, Diffusive or Intermediate regime?

- The measured value of the resistivity of MnBi (~15 $\mu\Omega\ cm$ at 4 K)
- The calculated density of states, $N_\uparrow = 0.446$ and $N_\downarrow = 0.425$ states/eV/cell
- Mean free path for majority ($\uparrow$) and minority ($\downarrow$) carriers from the Ziman formula

$$\sigma_{\uparrow(\downarrow)} = \frac{1}{3}e^2N_{\uparrow(\downarrow)}v^2_{F(\uparrow\downarrow)}\tau,$$

$$L_{\uparrow\downarrow} = v_{F\uparrow\downarrow}\tau$$

$$L_\uparrow \approx 20\ nm,\ L_\downarrow \approx 10\ nm$$

- Wexler’s formula for contact size, $R_c \approx \frac{4\rho L}{3\pi d^2} + \frac{\rho}{2d}$

$$d = 5\ to\ 15\ nm\ for\ 10\ \Omega < R_c < 100\ \Omega$$

- The transport is in the
  - Ballistic regime ($L > d$) for majority
  - Intermediate regime ($d \sim L$) for minority carriers

- Experimental values: ($P_T = 51-63\%$) with ballistic regime of transport
  - Theoretical values: Diffusive $P_{nv}^2 = 51-66\%$, Ballistic $P_{nv} = 28-36\%$

This is possible due to the fact that $P$ is sensitive to the interface and the termination of electrodes (there is substantial difference in electronic DOS of Mn and Bi at the Fermi energy). Bi states control the magnitude of $P$ ($P_{nv} = 55\%$ and $P_{nv}^2 = 76\%$, respectively)
Any role of spin orbit (SO) interaction in spin polarization?

- **Majority spin channel Without SO coupling**
- **Minority spin channel Without SO coupling**
- **Both spin channels with SO coupling**

- Electronic Band Structure: fully relativistic calculations of bulk MnBi in NiAs phase by tight binding LMTO method within local density approximation: Inclusion of SO does not significantly change the dispersion relationship at Fermi level. So, Fermi velocities and transport spin polarization would be only marginally affected by SO coupling.

- Calculations of density of states with and without SO coupling shows that there is no difference in the total DOS though there is slight band shift on the order of SO constant.
- This indicates that SO has no effect practically on our results.
- Calculations are performed using VASP.
The origin of large transport spin polarization: spin asymmetry of electronic bands

- DOS for majority and minority carriers at Fermi energy are ~0.45 states/ev/cell resulting vanishing $P_N = (N_{↑} - N_{↓}) / (N_{↑} + N_{↓})$.

- The origin of large $P_T$ measured in MnBi is due to the substantial spin asymmetry of the electronic bands near the Fermi energy.

- Projection of velocities along c axis gives the theoretical estimate of $P_{NV}^2$ as 66% and $P_{NV}$ as 36% which are found reduced to 51% and 28% for the velocity direction perpendicular to c axis. This implies that lower P are found in polycrystalline MnBi due to strong anisotropy in transport properties.

- Fermi velocities $v_F(↑(↓))$ are $1.2 \times 10^6$ and $0.6 \times 10^6$ m/s for the majority and minority bands, respectively.
Conclusions

A transport spin polarization of MnBi films was measured using the point contact Andreev reflection technique and values up to 63% are obtained, consistent with observations of a large magnetoresistance in MnBi contacts and the results of band-structure calculations.

In spite of almost identical densities of states at the Fermi energy in the majority- and minority-spin bands, the large disparity in the Fermi velocities results in a high transport spin polarization of MnBi.

Our experimental data and first-principles calculations show a nearly linear relationship between the values of $P_T$ and the magnetic moment (magnetization) of MnBi.
Thank you