Magnon scattering in single and bilayer graphene intercalates

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Magnon scattering in single and bilayer graphene intercalates

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Semi-classical Monte Carlo simulation is used to determine the effect of magnetic substance as intercalated layer in single layer and bilayer graphene intercalates on spin relaxation length. Spin relaxation lengths are studied with spin density matrix calculation under the effect of one magnon scattering mechanisms. Spin relaxation lengths are simulated and made comparisons by including magnon scattering with phonon scattering. The results are simulated with varying temperatures below Curie temperature. © 2012 American Institute of Physics.

I. INTRODUCTION

Ever since the experimental synthesis of graphene,1 there has been renewed interest in understanding the properties and application of graphene. It shows exceptionally high carrier mobilities2 and spin relaxation (or diffusion) lengths.3,4 These properties make graphene a possible candidate for future use in applications like superconductors and spin-transistors.5 The bilayer graphene has shown spin relaxation length of the order of a few micrometres,6 which is greater than what is observed in single layer. But both single layer graphene (SLG) and bilayer graphene (BLG) differ a lot in their electronic properties, dirac fermion like electronic transport, and absence of band gap in SLG,7 whereas the electrons show effective mass and electric field induced (and tuneable) bandgap in BLG.8 In fact, the E-K relationship in BLG is considered as parabolic,9,10 albeit a very low effective mass, which is $E = \frac{\hbar^2 k^2}{2m_{\text{eff}}}$. 

Apart from pristine graphene, a lot of research is being done around graphene intercalated with different substrates. Graphite intercalation compounds (GICs) are complex materials that are formed by insertion of atomic or molecular layers of different chemical species (called intercalating agent) between graphite interlayer spaces.12 This affects the interlayer distance, which in turn affects the electronic coupling between the layers.

It is of great advantage as the molecular, structural, electronic, and spintronics properties can be modified or controlled with the choice of proper intercalating agent. Graphene intercalated with Ca and Yb has shown remarkable superconductive properties,13,14 whereas potassium intercalation is finding its uses in Li and H2 storage and transport.15 Thus, graphene-based intercalation compounds would be an efficient method to modify the spintronics properties of single or bilayer graphene. There were a few success in synthesizing few layer graphene intercalates with intercalatants like I2 and Br2 (Ref. 16) but synthesis of FeCl3 is a real cornerstone.17 It is an obvious motivation that the magnetic nature of FeCl3 lattice will affect the spin transport properties of graphene electrons. Though the magnetic nature persists at a low temperature only, the study could still lay the path for future research in this direction. And as we show in our research, the spin relaxation length in bilayer graphene actually increases with the use of FeCl3 substrate, thus promising exciting avenues of research in this direction.

II. THE SPIN WAVE PARTICLE: MAGNON

Just as a phonon is a quasiparticle that characterizes the vibrational motion of every atom in the crystal, a magnon characterizes the electrons' spin structure in a crystal lattice. It carries a fixed amount of energy, lattice momentum and possesses a spin of $\frac{1}{201}$. In the wave picture of quantum mechanics, a magnon is a quantized spin wave.18 Spin waves are propagating disturbances in the ordering of magnetic materials. Fig. 1 shows the spin angular momentum carried by collective magnetic-moment precession.19

Spin devices primarily employ three processes-spin injection, spin transport, and spin detection. It is the second process-spin transport that is majorly affected by external scattering mechanisms. The injected electrons from source...
are coherent in the sense of having a common spin polarization direction. The ensemble undergoes different scattering mechanisms during its course of travel in the device, causing this average polarization to rotate several radians and finally undergo decoherence. The length over which this substantial decoherence takes place is referred to as the spin relaxation length in the literature. It is the spin relaxation length that we understand to be affected greatly by the ferromagnetic nature of FeCl$_3$ intercalant.

Since we use the semiclassical model of electron travel in our Monte Carlo simulation, to consider the effect of spin wave of the lattice of ferric chloride substrate, the quasiparticle magnon is utilized. The magnon scattering is an effect of presence of magnetic material alongside the graphene layer. Naturally, the effect needs to be studied below the Curie temperature of the material.

### III. MODELING MAGNON SCATTERING

The scattering mechanisms taken into account in our simulations are intravalley acoustic phonon scattering, surface roughness scattering, and polar optical phonon scattering. We consider a one magnon (talk about spin flip above) scattering process as described by Souto et al. for 2D quantum well systems. Graphene owing to its honeycomb sheet structure of carbon atoms is essentially a 2D sheet. For magnetic elements like Fe, Mn, and Cd, the s-d model describes the magnetic properties and hence can be used to determine electron scattering lifetimes for one magnon scattering. The magnons are assumed to be unconfined and follow an isotropic parabolic dispersion relation.

For an electron $i$ with energy $e_i$ in a 2D quantum well, the rate of spin flip is given by

$$
\frac{1}{\tau_{\text{flip}_i}} \approx \frac{\pi A (\alpha N_0)^2 S D_{\text{magn}}(T, \omega_{\text{mag}})}{\hbar N_0 L} \frac{e_i}{e^{\frac{-E_i}{k_B T}} + 1},
$$

where $\alpha N_0$ is the s-d exchange coupling constant for the substrate, which in our case is 0.22 eV, $S$ is the quantum spin number for Fe$^{3+}$, and $D$ is the density of states given by

$$
D_{\text{SLG}} = \frac{1}{\hbar \omega_F} \sqrt{\frac{g n}{n}},
$$

for single layer graphene.
for bilayer graphene \( (g \text{ is the degeneracy at brillouin zone of graphene, } g = 4) \), \( m_{eff} \) is the effective mass of electron, \( N_0 \) is the cation ion density, and \( M_{ocp} \) is the magnon occupation number

\[
M_{ocp} = \frac{1}{\left(e^{\hbar \omega_m/k_BT} - 1\right)}.
\]

The cation ion density depends on the lattice structure. In our case, since FeCl₃ follows HCP, iron atoms are at corners of unit cell and chloride atoms at face centers, the effective cation ion density is given by \( N_0 = 3/a^3 \), where \( a \) is the lattice parameter for our substrate.

During its scattering with magnon, the electron’s energy increases (or decreases) by the quanta of magnon’s energy if it is magnon absorption (or emission). The momentum final state of scattered electron is determined similar to the case of phonon scattering as essentially both magnons and phonons are bosons and have similar effects on momentum of electron with which they interact. But crucially the spin is flipped when a magnon is absorbed or emitted from the electron. This is represented in Fig. 2. The curie point of FeCl₃ is \( \sim 5 \text{ K} \). Hence the magnetic nature of the substrate plays a role only below this temperature.
IV. SIMULATION MODEL

Jacoboni et al.\textsuperscript{28,29} give comprehensive review of application of Monte Carlo technique for modeling spin transport. Important assumption made here is that all electron interactions are confined to the lowest subband. The scattering mechanisms employed are acoustic and optical phonon scattering. The detailed description of the model is provided in the previous works of Ghosh \textit{et al.}\textsuperscript{6,20,30} One limitation of the model is that it is incapable to perform at ballistic transport levels as we study diffusive transport only with Monte Carlo method. But for the temperature limits under our present considerations, graphene electrons never reach ballistic levels.

V. SIMULATION RESULTS AND DISCUSSION

The choice of temperature to run the simulation is 4 K. The simulations are run with the inclusion of magnon-electron interactions (with different magnon energies) and are compared with a scenario where no magnon scattering is present. Other dominant scattering mechanisms considered are phonon scattering, which consists of both acoustic and optical (both absorption and emission) phonons.

Figs. 3–11 show the spin relaxation length as a function of magnon energies for single layer graphene. Fig. 12 sums up the result and shows the variation observed in spin relaxation length as magnon energy increases. As observed from the figure, spin relaxation length reaches peaks at about

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FIG. 8. Total spin $|S|$ along channel length for magnon energy 4 meV.

FIG. 9. Total spin $|S|$ along channel length for magnon energy 5.2 meV.

FIG. 10. Total spin $|S|$ along channel length for magnon energy 7 meV.
3 meV and later saturates to original value. Table I shows the simulation results obtained for different magnon energy levels.

For bilayer graphene, Figs. 13–22 show the spin relaxation length as a function of magnon energies. Fig. 23 sums up the result and shows the variation observed in spin relaxation length as magnon energy increases. As observed from the figure, spin relaxation length reaches peaks at about 3 meV and later saturates to original value. Table II shows the simulation results obtained for different magnon energy levels.

The discussion on results can be broken down into three parts. At very low magnon energies, since the magnon scattering rate is very high, the net scattering rate also becomes very high. The dramatic decrease in the spin relaxation length at these energies can be understood with the help of increase in D’yakonov-Perel (DP) mechanism. As momentum scattering increases, the precession of spin of individual electrons also increases. Moreover, as the net internal electric field keeps on changing rapidly, the precession axis also keeps on changing direction rapidly.

But around the magnon energies of 3–4 meV, the scattering becomes comparable to other scattering mechanisms, notably the acoustic phonon scattering which is dominant at low temperature. In this case, the spin flip helps the ensemble to overcome the effect of momentum scattering and the net spin relaxation length increases. This conclusion is the starkest aspect of this work and can be attributed to the magnetic properties of intercalant FeCl₃ which assist the spin relaxation length to increase.

### Table I

<table>
<thead>
<tr>
<th>Magnon energy (meV)</th>
<th>Spin relaxation length (nm)</th>
<th>% change compared to no magnon</th>
</tr>
</thead>
<tbody>
<tr>
<td>No magnon</td>
<td>1020</td>
<td>-</td>
</tr>
<tr>
<td>1.5</td>
<td>115</td>
<td>-88.7</td>
</tr>
<tr>
<td>2</td>
<td>480</td>
<td>-52.9</td>
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<tr>
<td>2.5</td>
<td>960</td>
<td>-5.9</td>
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<tr>
<td>3</td>
<td>1290</td>
<td>+26.5</td>
</tr>
<tr>
<td>3.6</td>
<td>1160</td>
<td>+13.7</td>
</tr>
<tr>
<td>4</td>
<td>1050</td>
<td>+2.9</td>
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<tr>
<td>5.2</td>
<td>1000</td>
<td>-1.9</td>
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<tr>
<td>7</td>
<td>1030</td>
<td>+0.98</td>
</tr>
<tr>
<td>10</td>
<td>1025</td>
<td>+0.49</td>
</tr>
</tbody>
</table>

**FIG. 11.** Total spin $|S|$ along channel length for magnon energy 10 meV.

**FIG. 12.** Variation of spin relaxation length as magnon energy varies.
FIG. 13. Total spin $|S|$ along channel length for magnon energy 1 meV.

FIG. 14. Total spin $|S|$ along channel length for magnon energy 1.5 meV.

FIG. 15. Total spin $|S|$ along channel length for magnon energy 2 meV.

FIG. 16. Total spin $|S|$ along channel length for magnon energy 2.5 meV.
FIG. 17. Total spin $|S|$ along channel length for magnon energy 3 meV.

FIG. 18. Total spin $|S|$ along channel length for magnon energy 3.6 meV.

FIG. 19. Total spin $|S|$ along channel length for magnon energy 4 meV.

FIG. 20. Total spin $|S|$ along channel length for magnon energy 5.2 meV.
At higher magnon energies, phonon scattering takes over and the spin relaxation length again converges to the reference rate of scenario where no magnon scattering is present, as expected.

It is to be noted that the range of fluctuation is highly different in single layer and bilayer graphene. Whereas in the former, the simulations show an increment of 26.5% and decrement of 88% at appropriate magnon energy levels, in the latter, the increment and decrement are only 8% and 16% at similar magnon energy levels. This might suggest the more opposition of bilayer graphene towards the effects of magnetic intercalatants.
### VI. CONCLUSION

To summarize, our simulation results show, qualitatively, spin transport depends heavily on the magnetic properties of the substrate. When a magnetic substrate like iron is used below its curie temperature, it modifies the spin relaxation length in both graphene and its bilayer. Both in single layer and bilayer graphene, the spin relaxation length shows a peak at around 3 meV magnon energy. In single layer graphene, it is responsible for increase of about 26% in spin relaxation length, whereas in bilayer graphene its increase is around 8%.

The starkest conclusion is the increase that our simulation predicts. Further experiments are needed in this direction to confirm this. Further studies also needed to be done, so as to determine why bilayer graphene shows more opposition towards effect of magnetic intercalatants. This can be a boost to the bid of graphene as the future choice of spintronics material and can potentially direct the study of spintronics in graphene in a new direction in a sense that future experiments can determine the optimum magnetic substrate that maximizes the spin relaxation length.

**TABLE II. Spin relaxation length results and % change compared to reference as a function of magnon energy for bilayer graphene intercalate.**

<table>
<thead>
<tr>
<th>Magnon energy (meV)</th>
<th>Spin relaxation length (nm)</th>
<th>% change compared to no magnon</th>
</tr>
</thead>
<tbody>
<tr>
<td>No magnon</td>
<td>3280</td>
<td>...</td>
</tr>
<tr>
<td>1</td>
<td>2760</td>
<td>−15.85</td>
</tr>
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<td>2</td>
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<td>−5.18</td>
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<td>3530</td>
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</tr>
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<td>3470</td>
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</tr>
<tr>
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<td>+0.91</td>
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<td>7</td>
<td>3290</td>
<td>+0.3</td>
</tr>
<tr>
<td>10</td>
<td>3270</td>
<td>−0.3</td>
</tr>
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