A Rigorous Study of Nanoscaled Transistors Based on Single-Layer MoS$_2$

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Since the successful experimental isolation of graphene in 2004, ultra-thin two-dimensional structures are being widely studied as potential building blocks for future electronic devices. Among various two-dimensional materials, single-layer (SL) MoS$_2$ has attracted much attention. For a SL of MoS$_2$ a direct bandgap of 1.8 to 1.9 eV has been reported [1], which is suitable for various electronic applications. Recently, FETs based on SL MoS$_2$ with an $I_{on}/I_{off}$ ratio as high as $\sim 10^8$ and a sub-threshold swing of $\sim 70$ mV/decade have been achieved [2]. However, the reported mobility is below that of ultra thin body or strained Si and III-V materials. It is believed that extrinsic sources such as charged impurities (CI) [3] and inevitable Schottky contacts [4] limit the characteristics of devices based on SL MoS$_2$. High-$\kappa$ gate insulators, such as HfO$_2$, can reduce CI scattering effects and boost the mobility [3, 5], however, they can degrade the mobility due to remote phonon (RP) scattering [6]. The source of this scattering is in the surrounding dielectrics via long-range Coulomb interactions, provided that the dielectrics support polar vibrational modes.

To study electronic transport in SL MoS$_2$ we solved the NEGF equations self-consistently with the Poisson equation based on the box integration method. An effective mass of $m^* = 0.48m_0$ has been assumed for both longitudinal and transverse directions [7]. We have considered intrinsic electron-phonon interactions including the longitudinal acoustic (LA), the transverse acoustic (TA), the longitudinal optical (LO), and polar optical phonons (POP) with the parameters adopted from Ref. [7]. The mobility is calculated based on the method explained in Refs. [8, 9]. For device simulation we assumed a channel length of 20 nm, a 10 nm thick HfO$_2$ gate insulator, and a 50 nm thick SiO$_2$ substrate, see Fig. 1. In this study the dynamic screening of remote phonon modes stemmed from HfO$_2$ and static screening of charged impurities are included. Figure 2 shows the transfer and output characteristics in the presence of intrinsic phonon scattering. The results indicate a relatively high $I_{on}$.
of 9 mA/µm and a high $I_{on}/I_{off}$ ratio of about $10^7$, which are close to the ballistic limit. Low field phonon-limited mobility is evaluated to be 580 cm$^2$/Vs in good agreement with the result of Ref. [7]. The effect of high fields on the mobility and carrier velocity are depicted in Fig. 3. The significant drop in the mobility is due to increased polar and non-polar optical phonon scattering at high electric fields.

Figure 4 shows the effect of CI scattering and RP scattering for an average carrier density of $\sim 10^{13}$ cm$^{-2}$. By using a high-$\kappa$ insulator the CI scattering is suppressed which enhances the mobility. On the other hand, high-$\kappa$ insulators introduce RP scattering which in turn reduce the mobility. Therefore, at low CI concentrations the mobility for a device with SiO$_2$ as the top gate is higher than that with HfO$_2$. Figure 4 shows the evaluated mobility in the presence of intrinsic phonons (IP), CI, and RP (CI+RP) in good agreement with experimental results from Refs. [3, 10]. Table I compares the mean free path and the mobility for each scattering mechanism studied in this work. The results show that acoustic phonons play a more significant role in short channel devices than other intrinsic phonon modes. However, RP scattering due to a 30 nm high-$\kappa$ HfO$_2$ results in the smallest mean free path. The presented results can be used for appropriate selection of the gate insulator material for optimal device performance.

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**TABLE I**
The mean free path ($\lambda$) and low-field mobility ($\mu$) for each scattering source. RP scattering is calculated for a 30 nm thick HfO$_2$.

<table>
<thead>
<tr>
<th>Phonon Modes</th>
<th>$\lambda$ (nm)</th>
<th>$\mu$ (cm$^2$/Vs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LA+TA</td>
<td>35</td>
<td>923</td>
</tr>
<tr>
<td>LO</td>
<td>157</td>
<td>4161</td>
</tr>
<tr>
<td>POP</td>
<td>87</td>
<td>2316</td>
</tr>
<tr>
<td>RP</td>
<td>5.7</td>
<td>151</td>
</tr>
</tbody>
</table>

**REFERENCES**