Impurity- and remote-phonon-limited mobility in TMD monolayers

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The study of the low-field carrier mobility in monolayer transition metal dichalcogenides (TMDs) is the subject of great interest because of the potential applications of these materials. Whereas most of the studies have been focused on free-standing monolayers [1], in practical applications, these monolayers are supported by an insulating substrate and can also be gated. In this case, in addition to scattering with charged impurities, interactions with interface plasmon/optical-phonons (IPPs) [2], [3], [4] affect transport and these processes may have opposite effects. Specifically, high-κ insulators have been shown, experimentally [5] and theoretically [6], to enhance dielectric screening of the impurity scattering potential, an effect that improves the charge-transport properties. On the other hand, IPP scattering is stronger in the presence of high-κ insulators. Thus, one may ask how 'pure' do the TMD monolayers have to be for IPP to control transport and in what range of impurity concentration high-κ insulators improve the mobility.

Here, we address these questions by considering TMD monolayers in a double gate geometry, assuming a SiO_2 substrate and HfO_2 or hBN as examples of high- and low-κ insulators, respectively. The band structure, phonon dispersion, and scattering with the phonons of the TMD layer have been calculated using first-principles methods (Quantum ESPRESSO [9] and EPW [10]), accounting for the screening effects of the insulators as described in Ref. [4]. The dielectric continuum approximation has been used to deal with IPP scattering [4]. We have treated scattering with charged impurities in the TMD using the screened Coulomb potential in a double-gate geometry [6]:

$$\phi_Q = \frac{e^2 G_Q}{1 - e^2 G_Q^{(22)}(d,d)\Pi_{2D}(Q,\omega=0)} ,$$

where G_Q is the Fourier transform of the Poisson Green's function when the impurity is located at the center of the 2D layer [6]. The quantity $\Pi_{2D}(Q,\omega=0)$ is the electronic polarizability of the 2D layer given by Stern [7] extended to non-zero temperatures [8]. We show in Fig. 1 the scattering rate calculated using the first Born approximation and the scattering potential given by the above equation.

Our results show that the presence of high-κ insulator results in higher impurity-limited mobility (Fig. 2), as expected from the more effective screening. Figure 3 (top) shows that for the low-κ hBN, IPP scattering controls transport only when the impurity concentration is lower than the mid-10^{11} cm^{-2}, whereas for HfO_2 IPP scattering controls transport at any impurity concentration (Fig. 3, bottom). Finally, in Fig. 4 shows that the role of impurity scattering dominates at low temperatures.

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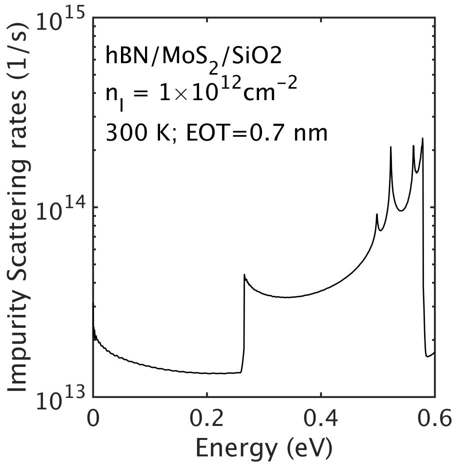

Fig. 1. Impurity scattering rates *vs.* electron kinetic energy in the hBN/MoS_2/SiO_2 stack calculated for an impurity concentration of 10^{12} cm^{-2} at 300 K. The insulators have been assumed to have an equivalent SiO_2 thickness of (EOT) 0.7 nm.

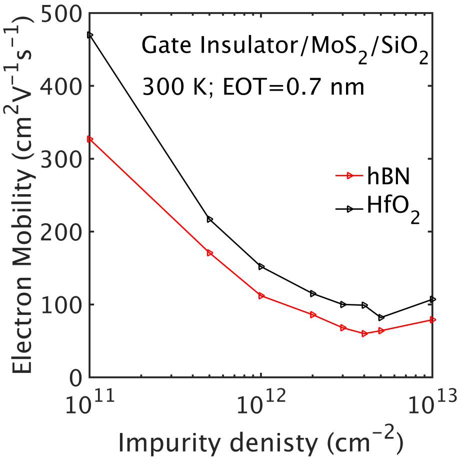

Fig. 2. Impurity-limited mobility *vs.* impurity density in the hBN/MoS_2/SiO_2 and HfO_2/MoS_2/SiO_2 stacks at 300 K.

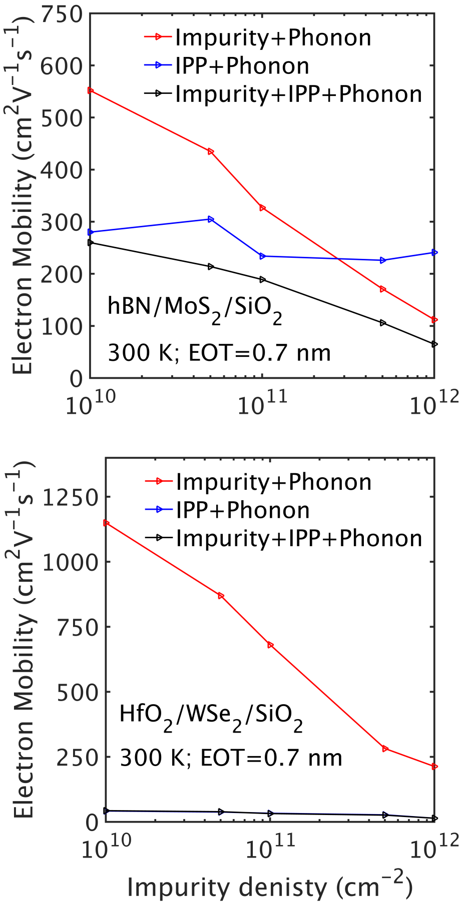

Fig. 3. Calculated electron mobility *vs.* impurity density for hBN/MoS_2/SiO_2 (top) and HfO_2/WSe_2/SiO_2 (bottom) stacks.

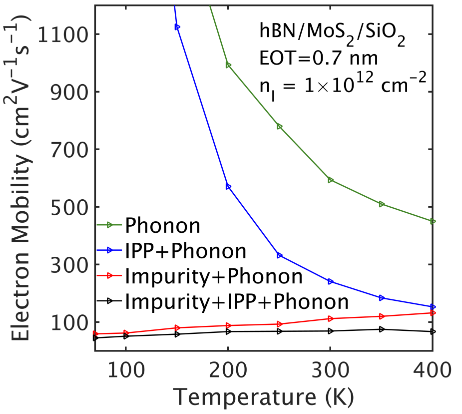

Fig. 4. Calculated electron mobility *vs.* temperature for hBN/MoS_2/SiO_2 stack. The Impurity-limited mobility increases with increasing temperature. This can be attributed to the temperature-independent screening by the insulator(s), by the increasing thermal carrier energy at high temperatures and the reduced scattering rates at high energy, as shown in Fig. 1.