Quantum Transport Study of Metal-TMD Contacts: Role of the Dielectric Environment

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ABSTRACT

We use non-equilibrium Green's Function (NEGF) quantum transport simulations to calculate contact resistance of metal contacted to TMDs and investigate the impact of non-uniform dielectric environment along the transport direction. We investigated five dielectric combinations and find that a low-κ near the metal edge gives lower contact resistances.

INTRODUCTION

Over the years, many strategies such as heavily doping the TMD to increase tunneling current, using low workfunction metals such as Scandium [1] have been developed to reduce contact resistance (R_c) in top contacts. Most recently, semi-metal contacts to MoS_2 have been demonstrated, where a record low R_c of 123 Ω-μm was achieved for Bi-MoS_2 system [2]. In terms of modeling, Density Functional Theory (DFT) has been used to study metal-TMD interfaces. However, the large computational burden involved in DFT presents a severe limitation in studying lowly doped TMDs, where the depletion length is large. Moreover, solving the Poisson equation and using the WKB approximation, some of us showed that the dielectric environment plays a critical role in side contacts [3].

In this paper we perform quantum transport simulations of a top and bottom contacted TMD. We shed light on the importance of the dielectric environment for these structures and identify the most promising dielectric setup that results in good contacts.

MODEL

We first generate a commensurate unit cell of two layers of metal and a TMD monolayer, where an interlayer distance of ~2.5 Å is obtained by performing structural relaxation calculations using VASP [4]. The commensurate unit cell is repeated along the transport direction (x) but to realize a top-contacted geometry, we remove the periodicity by applying a potential that eliminates a portion of metal above the TMD.

To perform self-consistent calculations, we apply a bias of 0.1 V to the right edge of the simulation domain. We model the electron density in the metal and TMD using (1) and (2) of Fig. 5. We model the TMD-contact current using the PETRA quantum transport code [5]. The self-consistent potential is used to construct the Hamiltonian in the NEGF formalism, where transmission is evaluated by applying quantum transmitting boundary conditions (QTBM). Equations for current and R_c are shown in Fig 5.

RESULTS

Fig. 1 shows the color plots of free charge density for four dielectric combinations. We see that systems with low-κ near the metal edge have smaller depletion widths. The band-diagrams shown in Fig. 2 reinforce this observation where the Schottky barrier height (SBH), measured at the metal edge, is lower for left-SiO_2 systems. The calculated R_c for five dielectric combinations is shown in Fig. 3, where left-low-κ systems have about 5 orders of magnitude lower R_c compared to their left-high-κ counterparts. In Fig. 4, we show the contact resistances as a function of left dielectric length (right dielectric being HfO_2). We observe an optimal length of at ~2 nm for which R_c is found to be the lowest.

CONCLUSIONS

Five different dielectric combinations are investigated for dual-metal TMD contacts. Having a low- κ near the metal edge was found to give low contact resistances.

REFERENCES

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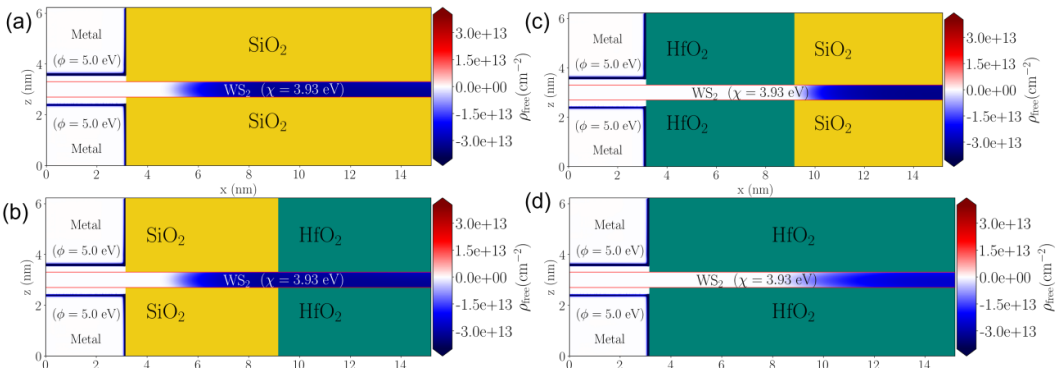

Figure 1. Color plots of free charge density for the four dielectric combinations. The TMD is *n*-doped to 1.73x10^{13} cm^{-2}. Configurations with low-κ environment closer to metal edge have smaller depletion widths.

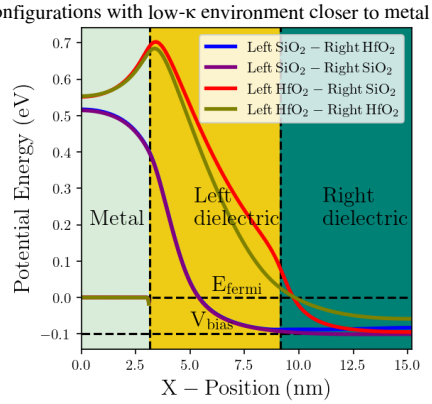

Figure 2. Band diagrams for the four different dielectric combinations, obtained by taking the cutlines (along the length of metal and TMD) of the mean of the self-consistent potential along the transverse direction (y). Systems with low-κ environment near the metal edge have lower barrier heights and smaller depletion widths.

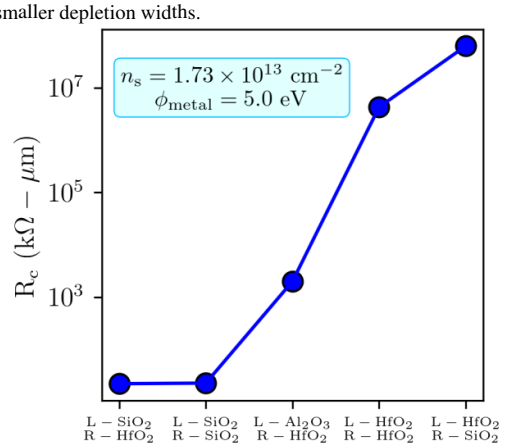

Figure 3. Calculated contact resistances for the four dielectric combinations. Left low-κ systems have the least contact resistances.

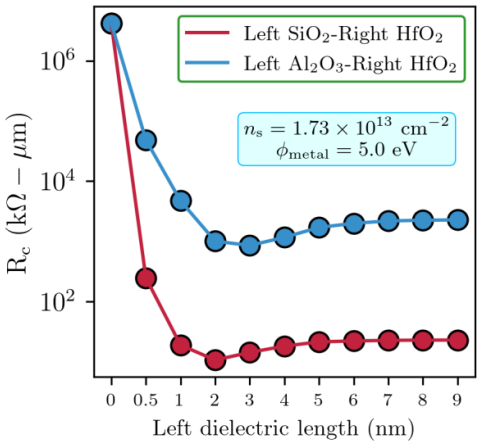

Figure 4. Contact resistance as a function of left dielectric length for metal-WS$_2$ system. For both cases, we observe an optimal left dielectric length of about 2 nm that gives the lowest R$_c$.

$$\rho = DOS_{\text{metal}} \times (E - \phi_{\text{metal}}) \quad (1)$$

$$\rho = \frac{m^* k_B T}{\pi \hbar^2} \ln\left(1 + e^{-\left(\frac{E-\chi-E_F}{k_B T}\right)}\right) \quad (2)$$

$$\nabla.[\epsilon(\mathbf{r})\nabla V(\mathbf{r})] = \rho[\mathbf{r}, V] + \rho_{\text{doping}}(\mathbf{r}) \quad (3)$$

$$[E\mathrm{M} - \mathrm{H} - \Sigma]\mathbf{c} = \mathrm{B} \quad (4)$$

$$I = \frac{2q}{h}\left(\int T(E)\left(f_L(E) - f_R(E)\right)dE\right) \quad (5)$$

Figure 5. Equations describing our methodology. (1) and (2) describe semiclassical modeling of free charge density in metal and TMD respectively. (3) is the non-linear Poisson equation used to find the potential self-consistently. (4) is then used to solve for the coefficients, **c**, of the injected modes at energy E, from which transmission coefficients are extracted [5]. And (5) is used to calculate current through the contact, using the transmission coefficients calculated above, from which contact resistance, R$_c$, is extracted.

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