Nonequilibrium Green's function method: Transport and band tail predictions in transition metal dichalcogenides

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INTRODUCTION

Transition metal dichalcogenides (TMDCs) based 2D materials appear to very promising materials for tunnel field-effect transistors (TFETs). [1], [2]. The intrinsic subthreshold slope (SS) of these devices is determined by exponentially decaying band tail states/Urbach tails below conduction and valence band edges which places a lower bound on SS. Though there have been few recent studies on calculating and extracting band tails using simple models and qualitative analysis [3], [4], a rigorous study based on atomistic approach is still lacking.

In this work, a physically consistent model to treat band tails through scattering self energies is developed. Polar optical phonon (POP) scattering, one of the dominant mechanisms in these devices is modeled through self energies. Band tail formation is demonstrated through atomistic simulations with only material dependent parameters. Variation of band tails with layer thickness is studied for 3 candidate TMD materials - MoS_2, WS_2 and WSe_2. As confinement increases, it is found that the Urbach parameter starts increasing due to an increase in the scattering strength.

METHOD DESCRIPTION

The atomic structures of all TMD layers modeled (i.e., MoS_2, WS_2 and WSe_2) are based on the relaxation calculations of the respective infinite number of layer systems in the 2H symmetry performed in the DFT tool VASP [5] with the self-consistent electronic model and the convergence criterion of 10^{-8} eV. The applied DFT model is based on the generalized gradient approximation utilizing the Perdew-Burke-Ernzerhof (PBE) functionals [6]. The electronic DFT Hamiltonian is transformed into an MLWF representation using the Wannier90 software with d orbitals for the metal electrons and sp3 orbitals for the chalcogenide electrons as the initial projection. The spreading of the Wannier functions is reduced iteratively until it converges to around 2A.

Transport calculations are then performed through the NEGF approach. NEGF is widely accepted formalism for nanoscale electronic, thermal and optoelectronic simulations [7], [8], [9] due to it's ability to consistently treat coherent and incoherent processes. Within the NEGF formalism, scattering is treated through the self-consistent Born approximation where the scattering self-energy is solved iteratively with the Green's function until convergence as shown in Fig. 1. Fröhlich coupling is used to model the electron-phonon interaction potential. Electrostatic screening is calculated through the Debye approximation. Static dielectric constants for respective layers are obtained from [10] and high frequency dielectric constants are obtained by using expression from [11] Above simulation methods have been implemented within the multipurpose nanodevice simulation tool, NEMO5 [12].

RESULTS

At room temperature, the band gap narrowing due to band tails is in the order of few k_BT. This can strongly alter performance of TFETs where band gaps play an important role in device behaviour. Through atomistic scattering simulation, one can directly observe such Urbach tails and extract the Urbach parameter as shown in Fig. 2. Electron-phonon Fröhlich coupling parameter is directly proportional to the phonon frequency and inversely to the difference of static and high frequency dielectric constant as shown below.

$$g_{FR} = \sqrt{\frac{e^2\hbar\omega_{LO}}{2\epsilon_o V}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_o}\right)}$$

With increasing layer thickness, dielectric constant of corresponding 2D material increases while the phonon frequency pretty much remains constant. This shows up as a decrease in the Urbach parameter from a monolayer device to bulk device as shown in Fig. 3. Phonon frequency of MoS_2 is the largest among the 3 materials (48 meV) and has the largest Urbach parameter as expected. WS_2 and WSe_2 having comparable phonon frequencies and dielectric constants have similar values and lower than MoS_2.

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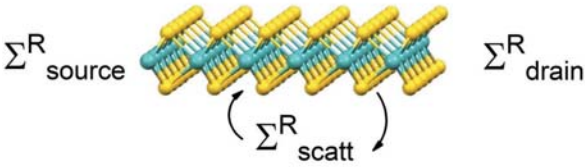

Fig. 1: Incoherent scattering is solved in NEGF through scattering self-energies defined in the device and iterated along with corresponding Green's function until convergence in a self-consistent Born scheme.

Conclusion

Band tails are important in characterizing the SS of tunneling devices. In this work, band tails for 3 TMD materials are calculated through an atomistic NEGF approach. It is shown that as the layer thickness increases, the Urbach parameter decreases due to decrease in scattering strength.

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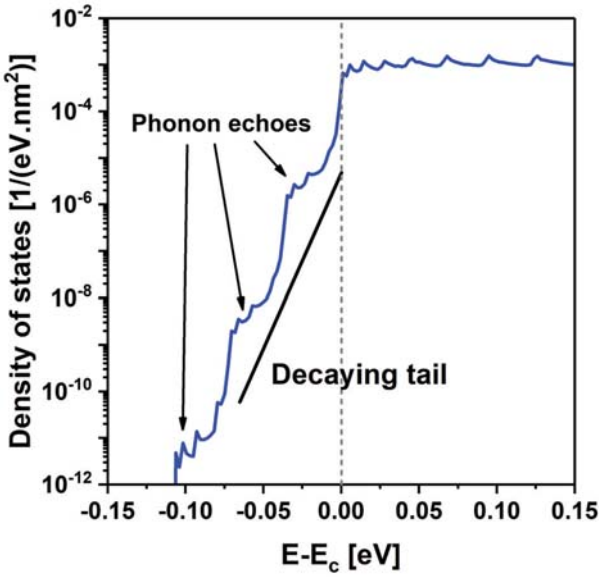

Fig. 2: Formation of band tails with exponentially decaying density of states obtained below conduction band edge. Slope of the decaying tail directly provides the Urbach parameter

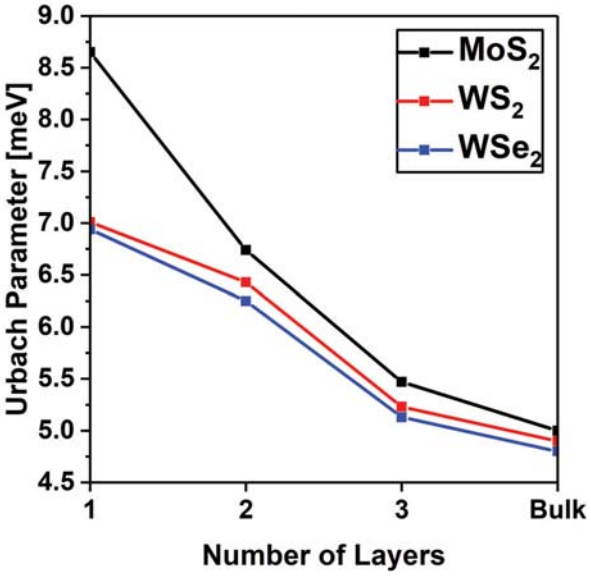

Fig. 3: Variation of Urbach parameter as a function of number of layers. MoS2 with a larger phonon frequency and relatively smaller dielectric constants has a larger Urbach parameter in comparison with WS2 and WSe2. Increasing layer thickness results in weaker electron-phonon interaction resulting in decreasing Urbach parameter.