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## The GPU Simulation of the MoS2 diode current characteristics

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Modeling of semiconductor carrier transport properties based on the drift-diffusion model is one of emerging activity of computational electronics. The p-n junction between materials with different type of conductivity can set up an internal electric field, which is responsible for separation of charge pairs electron and hole. The distribution of electric field in the depletion layer can be obtained by solution of Poisson's equation. Although this equation does not appear to have an analytical solution, numerical treatment offers a deeper comprehension of the structure, achieving a complete control on the various parameters and defining their role in the device operation.

In this paper, we implemented the GPU-based calculation of the p-n junction diode current simulation in the multiple parameter space. In particular, the parameter space is chosen as external voltage, diffusion coefficient and lengths. The GPU-based simulation has achieved the 2 times speedup compared to the CPU mode.

### Summary

In this paper, we implemented the GPU-based calculation of the p-n junction diode current simulation in the multiple parameter space. In particular, the parameter space is chosen as external voltage, diffusion coefficient and lengths. The GPU-based simulation has achieved the 2 times speedup compared to the CPU mode. We choose binary inorganic compound MoS2 for a p-n junction. Chemical structure simple molecular lattice is simulated by a program called a VESTA. We took MoS2 total length of the channel is 20 nm.

If we give V potential in p-n junction electron chemical potential difference will be  $\mu_L - \mu_R = qV$ . Density of state will be increased from the external voltage influence (Picture 1 Graph of Density of State) therefore change will be occurring in the density of electron charge.

The Poisson equation for a band bending in the depletion region given by following expression:

$$\frac{d^2\phi(x)}{dx^2} = -\frac{e}{\epsilon_s} (p-n+N_D-N_A)$$

In this case depletion region defined as:

$$\left\{ \begin{array}{l} p(x) = p_n + A e^{-x/L_p} + B e^{x/L_p} \quad (x > x_0) \\ n(x) = n_n + C e^{-x/L_p} + D e^{x/L_p} \quad (x < -x_0) \end{array} \right\}$$

And finally we will find from Shockley (or diode) equation total current:

$$J_p(x_0) = \frac{q}{A\tau_p} D_p \frac{p_n}{L_p} \left( e^{(eV_a / (k_B T))} - 1 \right)$$

We took three parameters:

$L_p$ - diffusion length

$p_n$ - carrier densities

$V_a$ - external voltage

to change the value in determining range to find the I(V) characteristic of p-n junction. This work allows calculating the current simulation in the accuracy of nano-meter scale.

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