The Impact of the Ring Shaped Valence Band in Few-Layer III-VI Materials on FET Operation

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ABSTRACT

Mexican hat shaped dispersions are relatively common in few-layered two-dimensional materials. In one to four monolayers of the group-III chalcogenides (GaS, GaSe, InS, InSe) the valence band undergoes a band inversion from parabolic to a Mexican hat dispersion [1]. This Mexican hat dispersion results in a singularity in the density of states at the band edge. This enhances the thermoelectric properties, however the effect on field effect transistor performance has not yet been investigated.

To evaluate the impact of this ring shaped dispersion on FET performance, we use a top of the barrier FET model. The physical gate length, effective oxide thickness and power supply voltage for the simulated devices are 12.8 nm, 0.68nm, and 0.3V respectively, following the low-voltage parameters described by Nikonov and Young [2]. The simulated device is shown in Fig. 1. To model the electrostatic potential along the channel of the device we solve a 2-D Poisson equation over the simulation domain. The density of states and density of modes calculated from the Mexican hat dispersion described in Ref. [1] are shown in Figs. 2 and 3, respectively. The density of modes is used as input for the current calculation. The performance characteristics of the devices are benchmarked using the 15nm node low-voltage criteria defined by Nikonov and Young [2] and compared to other devices.

The target ON-current for the low-voltage 15nm node of Si CMOS is 2uA/um. For the Mexican hat shaped dispersion the ON-current for doping density 1×10^{19} cm^{-3} is 20.4 times larger than the target ON-current. The ON-current is reduced as the doping density increases but it remains more than an order of magnitude larger for a doping density of 5×10^{20} cm^{-3}. The drain current versus gate voltage with $V_{dd} = 0.3$ V calculated for different doping densities is shown in Fig. 4.

We have also calculated the screened coulomb scattering time resulting from a Mexican hat dispersion and a parabolic dispersion from the Boltzmann transport equation as defined below

$$\frac{1}{\tau_\alpha} = \frac{N}{\hbar}\frac{e^4}{4\epsilon^2}\int_0^{2\pi}\sum_\alpha \frac{D(\epsilon_\alpha)}{\sqrt{q_0^2+\beta^2}}\cdot\left|1-\frac{\mathbf{v}(\mathbf{k}_\alpha).\mathbf{v}(\mathbf{k})}{v^2(k)}\right|$$

where α is the number of bands crossing $\mathbf{k}$, N is the number of charged impurity scatterers per area, D (ϵ_α) is the density of states, β is the transition wave vector, and q_0 is the screening factor. As shown by Fig. 5, the room temperature relaxation time for the Mexican hat dispersion is generally longer than that resulting from a parabolic dispersion. This result can be understood from the momentum dependence of the matrix element. In the Mexican hat dispersion, larger momentum transfer is required for backscattering. From the calculated relaxation times, we will determine the effect of the finite mean free paths on the FET performance.

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[2] D. E. Nikonov and I. A. Young, "Overview of beyond-cmos devices and a uniform methodology for their benchmarking," *Proceedings of the IEEE*, 2013.

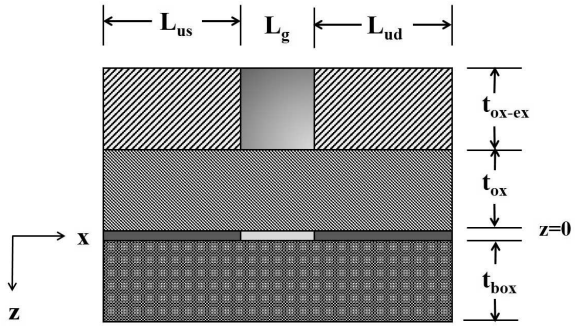

Fig. 1. Cross section of the device that was used for simulation. The dimensions used are $L_g = 12.8$ nm, $L_{us} = 60$ nm, $L_{ud} = 60$ nm. The substrate is SiO_2 ($t_{box} = 10$ nm) and the gate dielectric is HfO_2 ($t_{ox} = 4.36$ nm) with dielectric constant of 3.9 and 25 respectively. The oxide extension shown is SiO_2 (t_{ox-ex}) which is 6 nm. The channel is undoped and we have considered an effective mass of the channel as 0.4 which is the effective mass of GaS from ab-initio calculation.

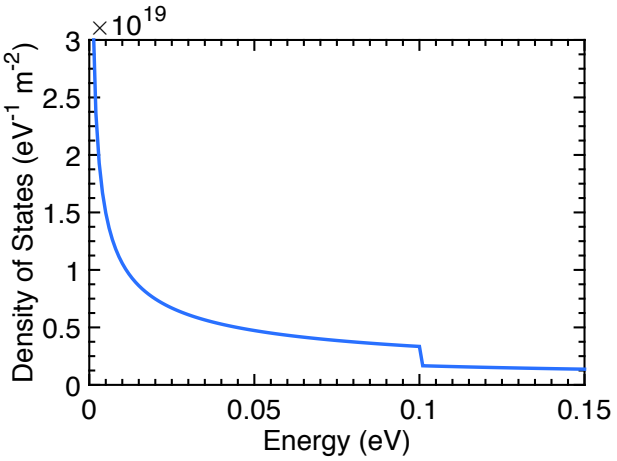

Fig. 2. Density of states calculated from the analytical model of Ref. [1] using an effective mass 0.4 and ϵ_0 = 0.1 .

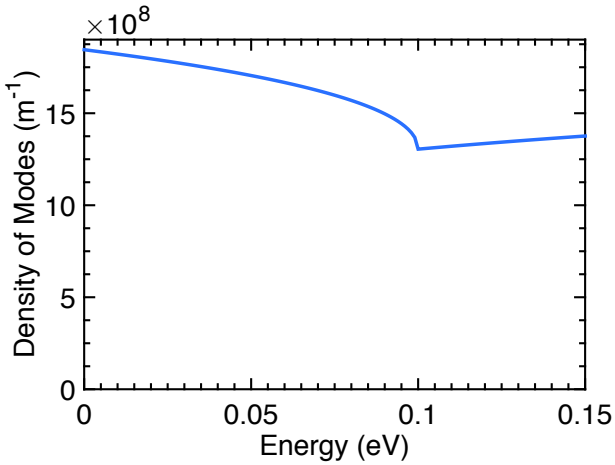

Fig. 3. Density of modes calculated from the analytical model of Ref. [1] using an effective mass 0.4 and ϵ_0 = 0.1 .

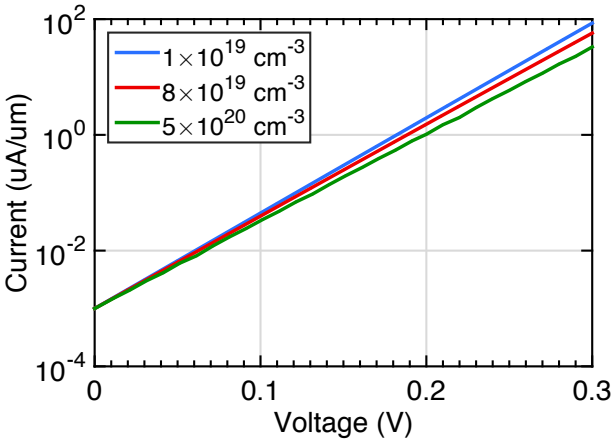

Fig. 4. Current versus gate voltage with $V_{dd} = 0.3$ V for different source and drain doping densities.

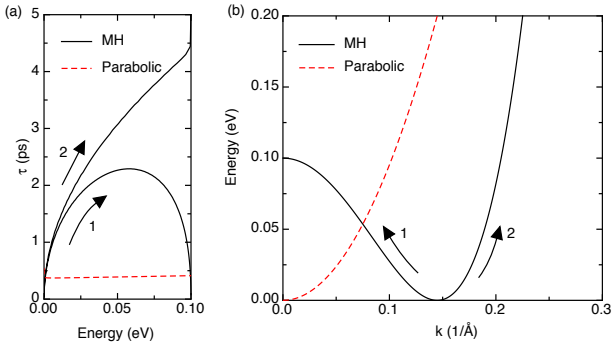

Fig. 5. (a) Momentum relaxation times calculated from Coulomb impurity scattering and (b) energy-momentum relations comparing parabolic and Mexican hat dispersions. The relaxation times for states on the two different branches of the Mexican hat dispersion are labeled in (a). The density of impurity and electron density used are $1 \times 10^{-5} \mathring{A}^{-2}$ and 1×10^{-11} cm^{-2} respectively.