

# Numerical study of p-type InSb and GaSb nanowires

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## 1. Abstract

III-V nanowires (NWs) have attracted extensive research interests in recent years because of their unique physical properties, being recognized as promising building blocks for the next generation of electronics and photonics. Most of the works up-to-date are, however, focused on n-type devices where materials such as InAs or InGaAs have already demonstrated impressive performance. Nevertheless, for the practical implementation of CMOS circuits based on NWs, p-channel FETs are mandatory. Several materials are currently being investigated as technologically relevant p-type semiconductors. In particular, increasingly more attention has been focused on InSb and GaSb NWs owing to their excellent hole transport properties. In this work we study the electrostatic properties of traditional p-type NWs based on Si and Ge compared to III-V materials.

## 2. Numerical Simulator

Traditionally, the effective mass approximation (EMA) has been used to describe the Conduction Band (CB) in NWs. However, this method fails in the description of the Valence Band (VB) in group IV (Si, Ge) and III-V compound semiconductors due to the coupling of the different subbands forming the VB (Heavy Holes, Light Holes and Split-Off). To analyze it, we have developed an eight-band  $k\cdot p$  model which accounts for the coupling between the VB and the CB, an effect that must be considered when studying small gap materials. Moreover, this eight-band  $k\cdot p$  has been self-consistently solved with the Poisson equation in order to achieve an accurate electrostatic description of the NW.

## 3. Results and Discussion

Otherwise stated, in this study we have considered a square NW with 5nm width, oriented along the [111] direction. In addition to InSb and GaSb, we have also included Si and Ge as channel materials in order to benchmark the performance of III-V materials against that of traditional semiconductors. Fig. 1 shows the bandstructure at a gate overdrive voltage of 0V (top) and -0.4V (bottom). The energy is referred to the VB edge, and the Fermi level ( $E_F$ ) is depicted by a dotted grey line. The threshold voltage ( $V_T$ ) is calculated from the maximum of the second derivative of the charge with respect to the gate voltage [1]. A quite different scenario is observed between Si and the other three channel materials. The former shows a large number of

bands per unit energy with a lower curvature, which corresponds to a higher DOS and higher effective mass as compared to the latter. The increase of the overdrive voltage,  $V_G - V_T$ , from 0V to -0.4V provokes, for all the semiconductors, a reduction of the energetic separation between the first and second subbands, which is more accused for Ge. The effective mass has been evaluated for these devices as a function of the gate voltage, using the mean transport effective mass expression presented in [2], Fig. 2. As can be seen, the results are consistent with the band structure shown in Fig. 1, with Si having roughly  $\sim x2.5$  higher effective mass than the other three materials.

Fig. 3 presents the gate capacitance behavior as a function of the gate overdrive voltage. As shown, the capacitance behavior of III-V NWs outperforms that of Ge ones, holding the comparison with Si devices, despite their small effective mass.

Finally, we have studied the hole distribution through its centroid [3], which is depicted in Fig. 4 as a function of the gate overdrive voltage for each of the materials considered in this work. Its behavior is similar in the subthreshold regime, where the charge gets close to the device center. Nevertheless, when increasing the inversion charge (i.e., the overdrive voltage), the centroid of III-V NWs is higher than that of Ge and Si devices, thus resulting in a larger average distance between the charge and the semiconductor/insulator interface. This fact suggests a reduced influence of surface roughness in the hole mobility, which may be critical for these ultra-scaled devices.

## 4. Conclusion

A numerical simulator that self-consistently solves the Poisson equation and the eight-band  $k\cdot p$  method in the cross section of a 5nm square NW has been developed. A comprehensive study of the electrostatic performance of this device has been carried out focusing on p-type channels and four different materials: Si, Ge, InSb and GaSb. Our results indicate that, in spite of their lower effective mass and smaller density of states, GaSb and InSb NWs hold the comparison with Si and outperform Ge in terms of gate capacitance and inversion charge. The good electrostatic performance combined with the expectation of superior transport characteristic place GaSb and InSb as attractive alternatives for p-type CMOS logic based on NWs.

## Acknowledgement

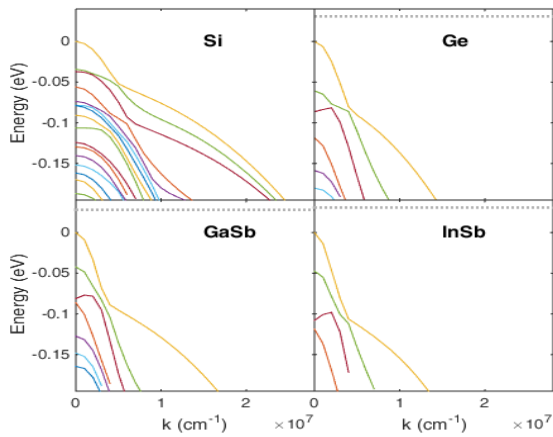
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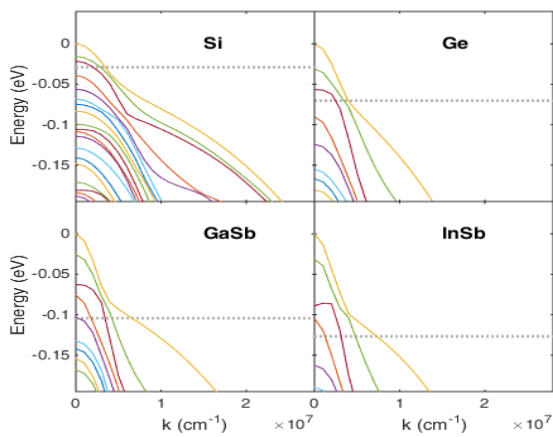
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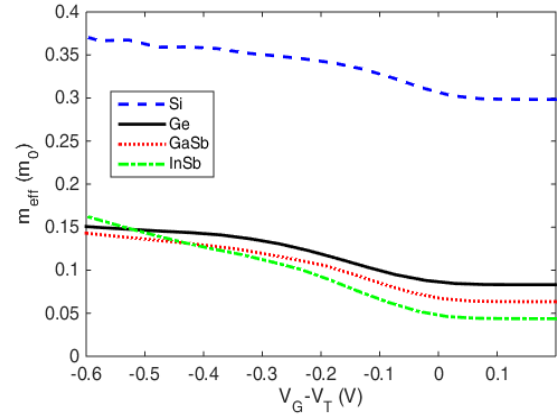
**5nm sq [111] NW -Bandstructure at  $V_G - V_T = 0.0V$**



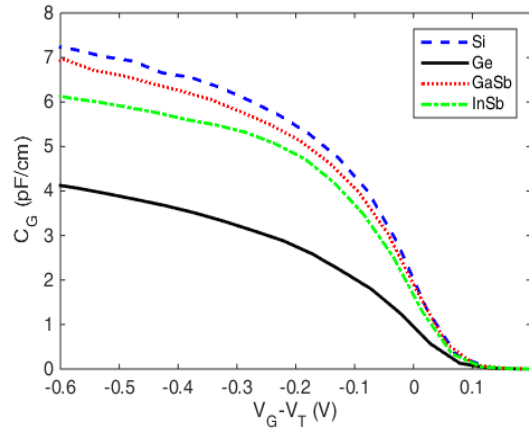
**5nm sq [111] NW -Bandstructure at  $V_G - V_T = -0.4V$**



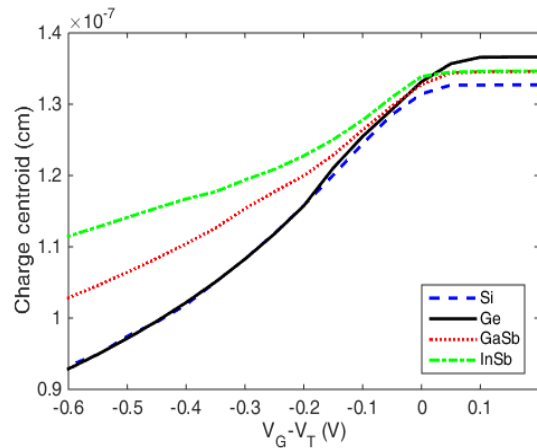
**Fig.1.** Bandstructure for a 5nm NW and four materials at a gate overdrive voltage of 0V (top) and -0.4V (bottom). The energy is referred to the maximum of the VB, and the Fermi level is depicted by a dotted grey line.



**Fig.2.** Effective mass as a function of the gate voltage overdrive voltage ( $V_G - V_T$ ) for a square [111]-oriented NW with different materials.



**Fig.3.** Linear gate capacitance  $C_G$  (pF/cm) as a function of the gate overdrive voltage ( $V_G - V_T$ ) for a 5nm square NW.



**Fig.4.** Charge centroid as a function of the gate overdrive voltage ( $V_G - V_T$ ) for a square NW with 5nm width.