Effect of Strain on Electronic Transport in Silicene Nanoribbon using Tight Binding Model

Anshuman Shukla, Rajesh C. Junghare and Ganesh C. Patil

Centre of VLSI and Nanotechnology, Visvesvaraya National Institute of Technology Nagpur,Nagpur - 440010, Maharashtra, INDIA,
Tel: +91 712 280 1591, Email:ganeshcpatil@cvn.vnit.ac.in

ABSTRACT

In this paper, we investigate the effect of strain on silicene nanoribbon by using tight binding model.Using appropriate models for silicene, we apply a variable strain to Silicene nanoribbon and analyzed the impact of strain on the transfer characteristics of the silicene nanoribbon field effect transistor. Further, we compared the variations in off-state leakage current (I_{OFF}) and the on-state drive current (I_{ON}) with variation in strain. It has been found that, as the strain increases the $I_{OFF}$of the device decreases.

Keywords: **Silicene, tight binding model, NEGF, strain, 2D Semiconductors**

1 INTRODUCTION

The discovery of graphene in the first decade of 21st century lead to a new era of two dimensional (2D) semiconductors.The 2D semiconductors not only have excellent mobility and long mean free path, butcan also be used for low power applications. These characteristics allows near ballistic transport in 2D semiconductors. Silicene, a hexagonal analogue of graphene [See Fig 1(a)] is one of the promising emerging material.Further, siliceneis convergent with the current silicon based semiconductor industry.Unlike graphene, silicene has a buckled structure [See Fig. 1(b)], in which the buckling height can be varied by applying the perpendicular electric fields.

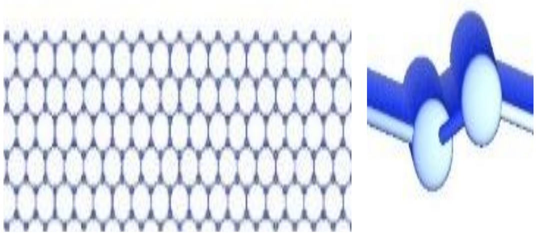

Fig.1. (a) Silicene nanoribbon top view. (b) silicene nanoribbon side view

One of the major problem faced by 2D semiconductors is their zero band gap, which proves to be a major hindrance to the transistor operation. An application of strain can open a tunable band gap in 2D semiconductors. Naumis et al. did strain analysis on 2D semiconductors using first principle approach [1]. Although Lin et al. proposed tight binding analysis on strained silicene, this study explores the material physics using the first principles [2]. Despite tight binding models on silicene have been reported in the literature [3-4], to the best of our knowledge the strain effect on silicene has not been studied from device perspective. In this paper, we explore the effect of strain on the electronic transport in silicene nanoribbon field effect transistor using tight binding model.

2 SIMULATION SETUP

The structure of the field effect transistor is shown in Fig.2 with armchair silicene nanoribbon as channel material. The width of source, drain and channel is of 10nm each.The oxide region has a width of 2nm. The chirality of the silicene nanoribbon is n=6. The device is simulated using NanoTCAD ViDES simulator[5].

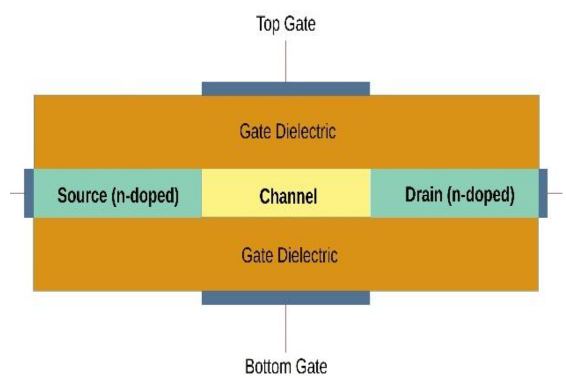

Fig.2. Device structure used in simulations

The simulator uses NEGF approach to solve equations self consistently. The Green's function is given as

$$G(E) = [EI - H - \Sigma_S - \Sigma_D]^{-1}, \quad (1)$$

where, H is the channel Hamiltonian and Σ_S *and* $\Sigma_D$are source and drain self- energies respectively[6-7].

The application of strain results in change in the lattice constant, buckling height and Fermi velocity, which in turn changes the hopping parameters (t_{hop}) of the silicene nanoribbon.The variation in t_{hop} is expressed as

$$t_{\text{hop}} = \frac{2v_{\text{F}}}{\sqrt{3}a_{\text{o}}} \qquad (2)$$

where,$a_{\text{o}}$is the lattice constant and v_{F} is the Fermi velocity. The drain current and the bandgap has been computed using the equations expressed in [8-11]. Further, the simulations have been carried out for both compressive and tensile strain applied to the silicene nanoribbon.

3 RESULTS

Fig. 3 shows the variation of drain current (I_{D}) as a function of gate-to-source voltage (V_{GS}). From Fig. 3 it can be clearly seen that, for lower V_{GS} values due to compressive strain, the I_{DS} is higher whereas at higher V_{GS} values due to the tensile strain I_{D} reduces. This variations in I_{D} is also being observed from the log I_{D} verses V_{GS} characteristics shown in Fig. 4. The increase in I_{D} at lower V_{GS} is mainly because of the smaller bandgap, which results in larger leakage current.

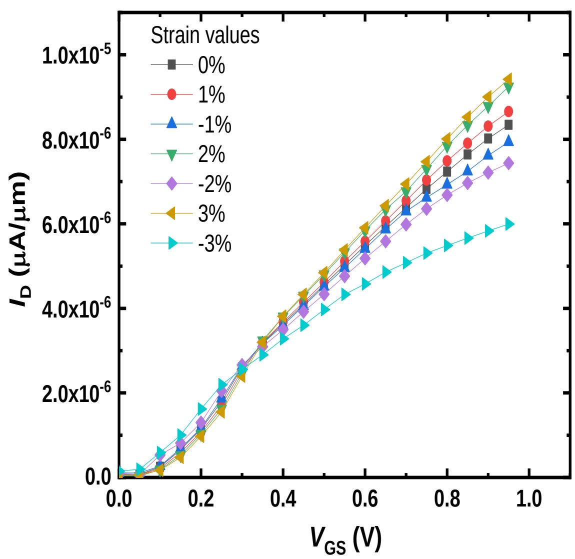

Fig.3. I_{D} vs V_{GS} characteristics for silicene nanoribbon at various strain values. $V_{\text{DS}} = 0.3$V.

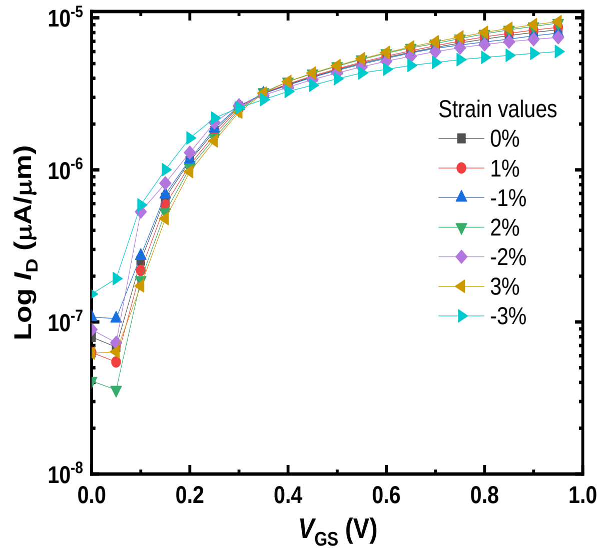

Fig. 4 Log I_{D} vs V_{GS} characteristics for silicene nanoribbon at various strain values. $V_{\text{DS}} = 0.3$ V.

Fig. 5 and Fig. 6 shows the transmission characteristics in the off-state and the on-state respectively, which clearly explains the variation in $I_D$verses V_{GS}. Furthermore, from Fig. 6 it can be seen that as the strain increases, the tunneling also increases. In this work the on-state drive current (I_{ON}) has been extracted at V_{GS}= 1 V and drain-to-source voltage (V_{DS}) = 0.3 V whereas the off-state leakage current (I_{OFF}) is extracted at V_{GS}= 0 V and V_{DS}= 0.3 V. It has been found that the $I_{\text{ON}}/I_{\text{OFF}}$ of the silicene transistor is ~10^2 for all the strain values.

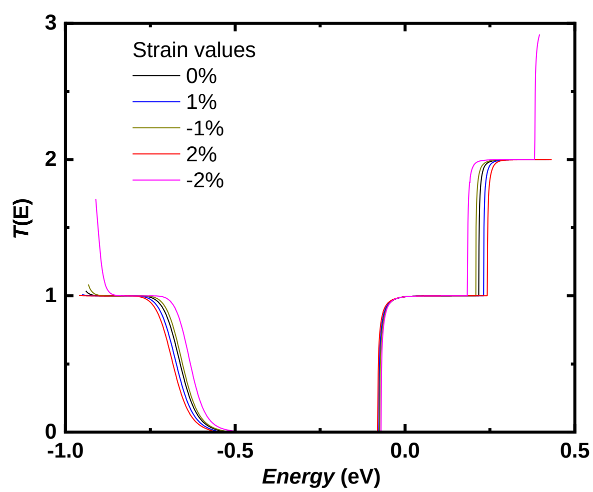

Fig. 5 Transmission parameter for silicene nanoribbon at various strain values. $V_{\text{GS}} = 0.15$ V.

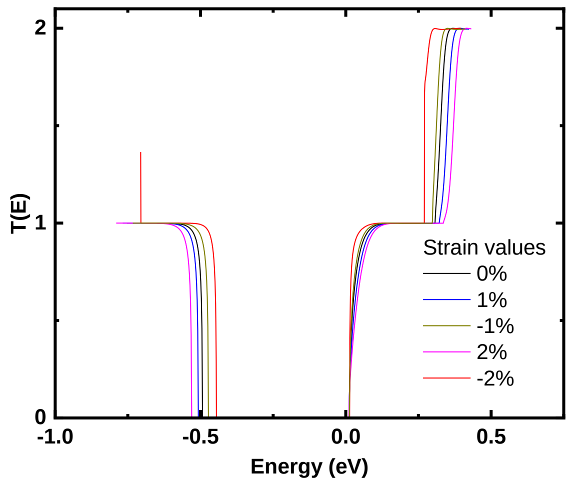

Fig. 6 Transmission parameter for silicene nanoribbon at various strain values. V_{GS} = 0.6 V

Furthermore, from Fig. 7 it can be seen that, at each value of strain there is ~10% increase in the bandgap, which is consistent with the predicted models for strain analysis on silicene [2]. In addition to this, we also observed that higher strains produce higher I_{ON}.

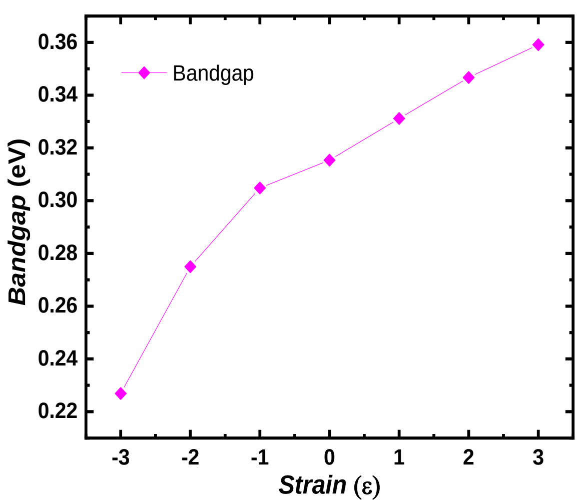

Fig. 7 Variation of obtained bandgap as a function of strain values for silicene nanoribbon

4 CONCLUSION

In this work the impact of strain on the silicene nanoribbon based field effect transistor has been analyzed. It has been shown that, increasing the strain on the silicene nanoribbon reduces the off-state leakage current and improves the on-state drive current of the field effect transistor. This clearly shows that, by increasing the strain on silicene nanoribbon improves the I_{ON}/I_{OFF} ratio of the device significantly. This improvement in $I_{ON}/I_{OFF}$is mainly because of the change in the transmission parameter and the bandgap of the silicene nanoribbon.

5 REFERENCES

[1] Gerardo G Naumis et al, *Rep. Prog. Phys*. vol. 80, pp. 096501, 2017.

[2] Xianqing Lin et al, *J. Phys.: Conf. Ser.* 491 012005, 2014.

[3] Roome and Carey, *ACS Appl. Mater. Interfaces* vol. 6, pp. 7743- 7750, 2014.

[4] Lian, C., Yang, Z., & Ni, J., *Chem Phy. Letters*, vol. 561, pp. 77-81, 2013.

[5] G. Fioriand G. Iannaccone,"Code for the 3D Simulation of Nanoscale Semiconductor Devices, Including Drift-Diffusion and Ballistic Transport in 1D and 2D Subbands, and 3D Tunneling", *J. Comp. Electron.*, vol., pp.63-66, 2005.

[6] Bhubon Chandra Mech, SumitSaha, Saddam Hussain, and Jitendra Kumar,*Proceedings of the 17thIEEE InternationalConference on Nanotechnology*, Pittsburgh,USA, July 25-28-2017.

[7] S. Datta, "Nanoscaledevicemodelling : the Green'sfunctionmethod", *Super lattices Micro struct.*, vol. 28, pp. 253-278, 2000.

[8] SeymurCahangirov, Hasan Sahin, Guy Le Lay, and Angel Rubio, *Introduction to Physics ofSilicene and other 2D Materials*,SpringerInternational Publishing AG 2017.

[9] S. Bruzzone, G. Iannaccone, N. Marzari and G. Fiori, "An open Source MultiscaleFramework for the Simulation of Nanoscale Devices," *IEEE Trans. Elect. Devices*, vol. 61, no. 1, pp. 48-53, 2014.

[10] Z.Shao ‘,X. Ye, L. Yang, and C.Wang, "First-principles calculationof intrinsic carrier mobility of silicene,"*Journal of Appl. Phys*., vol. 114, pp. 093712-1-093712-3, 20.

[11] L C L. Y. Voon, A Lopez-Bezanilla, J. Wang, Y. Zhang, and M. Willatzen, "Effective Hamiltonians for phospherene and silicene,"*New J. Phys.*, vol. 17, pp. 025004-1-025004-10, 2015.