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Current saturation and kink effect in zero-bandgap double-gate silicene field-effect transistors

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ABSTRACT

Double gate silicene field effect transistor is investigated using Density Functional Theory (DFT) and Non-Equilibrium Green's Function (NEGF) formalism. The results suggest that with an increase in gate bias, bandgap is introduced in silicene which results in reduction in device current. The increase in silicene bandgap is also related to the reduction in channel length. It is observed that drain to source current (I_{DS}) saturates on increasing drain to source voltage (V_{DS}). On increasing V_{DS} beyond saturation region, at some value of V_{DS} kink effect is seen which is due to switching in the type of carriers at the drain end due to ambipolar channel. Transconductance (g_m) is seen to reduce with reduction in channel length, however, g_m improves with reduced oxide thickness due to better gate controllability. The output characteristics do not change much with oxide thickness.

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1. Introduction

In order to follow the Moore's Law along with the purpose of achieving higher performance, the device technology has been scaled down tremendously [1]. In past several decades there is a continuous reduction in FET dimensions. Today the conventional 3D transistors are encountering various performance challenging issues of short channel effects such as punch through, sub-threshold leakage, static power dissipation etc [2]. Therefore, to increase the performance by scaling the device will not be sufficient enough, instead the efforts must be made in improving the electrical performance of the scaled device as well. In electronics, the progress is governed by the motto of "smaller, faster, cheaper" and that the device scaling still follows Moore's Law [3].

Only from the last decade in order to mitigate the short channel effects arising from scaling the devices, demand arises for principally different and new semiconductor materials beyond 3D silicon. This principally new material system should also be compatible with the existing CMOS technology. This is the main reason for the evolution of next generation 2D material based FETs.

Basically, channels made up of 2D materials are single atom thick layer or the stacking of these layers in different ways with overall thickness less than 1 nm. If we reduce the thickness of bulk 3D materials to form Ultra Thin Bulk (UTB) semiconductors then this will lead to charge carrier scattering because of the dangling bonds, undesirable phonon coupling and the interface states are created when the deposition of source/drain and gate dielectric takes place over the semiconductor [4]. Whereas in 2D FETs, as the channel is atomically thin, the carriers are confined only in two dimensions and therefore gate

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voltage influences them uniformly. This will lead to the elimination of leakage currents resulting in improved device performance with reduced static power dissipation [2].

As 2D materials possess the properties of high surface to volume ratio, mechanical flexibility, optical transparency and excellent electrostatic control they are best suited for advanced and flexible nanoelectronics and also for highly sensitive sensors [5]. Graphene was the first two-dimensional material which was investigated thoroughly and a FET with highly stable graphene channel was reported in 2004 by Novoselov and others [6]. Graphene possess honeycomb lattice structure with sp^2 bonded carbon atoms in two-dimensional planar sheet. Due to high carrier mobility and high saturation velocity graphene draws huge attention from the researchers [7]. Graphene also exhibits zero gap at the Dirac points [8] which limits the application of graphene as a channel for FETs. This raises the necessity of further exploration for some new materials in the field of 2D semiconductors with electrical properties similar to graphene but provides much more bandgap tuning in comparison to graphene.

Silicene is a two-dimensional material and a silicon analogous of graphene [9]. Silicene was mostly unnoticed until the fabrication of silicene nanoribbon was reported on silver substrate by Kara and others in 2009 [10]. Silicene possess the similar electrical properties as that of graphene, but with silicene the additional advantage is that it can make fabrication process much of commercial reality due to its natural compatibility with the present silicon technology. The first Silicene field effect transistor has been reported in 2015 by D. Akinwande and others [11]. Silicene is been considered as an alternative to post silicon industry and other 2D materials ever since its first successful synthesis. Silicene exhibits similar honeycomb lattice structure as that of graphene. This similarity is due to the fact that C and Si are elements of same group in the periodic table. For Si sp^3 hybridisation is much more energetically favourable as compared to that of C which favours sp^2 hybridisation. This is due to the larger ionic radius of Si atoms [12]. Silicene is slightly buckled as compared to graphene which exhibits planar structure [8,12]. The two sublattices in honeycomb silicene shows out of plane buckling with a vertical separation of $\Delta = 0.04$ nm from each other [3]. Such buckling provides a better control over the sublattice-asymmetric bandgap and electron dispersion in silicene [12]. Due to buckling, silicene exhibits higher spin-orbit coupling compared to graphene. Carriers in silicene also possess almost similar fermi velocity as in graphene [13]. Bandgap opening in silicene is much easier than graphene due to absence of strong π-bonds which makes structure of silicene more flexible than graphene [8]. For improving electronic and magnetic properties as well as bandgap opening in silicene different mechanisms have been explored which includes structural [13–17] or chemical modifications [18–20], substrate coupling [9,21], application of vertical electric field to the silicene layer [8,12,22]. Free standing silicene exposed to air is not stable, therefore it is not feasible to use the wet transfer technique for fabrication of silicene devices and thus a new technique is devised for the fabrication of silicene known as 'Silicene Encapsulated Delamination with Native Electrodes' (SEDNE) [8,23]. As the band diagram of silicene exhibits Dirac Cone like structure, it possesses massless Dirac fermions. This provides higher carrier mobility of the order of 10^3 cm^2 V^{-1} s^{-1} including electron phonon scattering [23]. This fascinates silicene for the fabrication of high speed switching devices. If silicene is used as a channel in field effect transistors then it is possible to achieve ultrahigh speed in THz frequency range [9]. Silicene also possess other properties such as chiral superconductivity, quantum spin hall effect (QSHE) [8] and good thermal stability which makes it a promising two-dimensional material to be explored further for future nanoelectronic devices [24]. It is therefore of interest to investigate silicene as a channel in field effect transistors. In this paper silicene FET is investigated.

2. Simulation method and setup

In this paper, we use DFT and NEGF to solve Schrodinger's equation and find current through self-consistent simulations. In this work, NanoTCAD ViDES [25] is used for simulations. This section provides a brief review of the complete simulation process used to investigate silicene field effect transistor. Ab initio method is used to compute fundamental quantities such as electron affinity, metal work function, scattering rate and energy dispersion relations (used for extraction of energy gap and effective mass). Density functional theory (DFT) efficiently predicts the density of states, as well as the structural properties of solids and molecules [26]. Electron density is uniquely determined from the given external potential [27]. For accurate computation of energy barriers or energy gaps, GW approximation is used. Schrodinger equation within the Green's function formalism in GW approximation is expressed as

$$\left[-\frac{\hbar^2}{2m_0}\nabla^2 + U_L(r) + V_H(r)\right]\psi_i(r) + \int dr' \sum\left(r, r'\right)\psi_i\left(r'\right) = \varepsilon_i\psi_i(r)$$

$\sum(r, r')$ is the self energy which is solved by self-consistent iterative scheme and is computed as

$$\sum = \text{iGW}$$

where W is a function accounting for screened Coulomb interaction and G is the Green's function of the many body systems.

There is an upper limit to the use of DFT up to few hundred atoms only, investigation for the systems larger than this is prohibitive. This is because the complexity in DFT increases as N^3, where N is the total number of orbitals considered. Then to investigate larger systems requires an alternative approach of defining Hamiltonian for the considered material. In this

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