Solid-State Electronics 114 (2015) 23–29

Contents lists available at ScienceDirect

Solid-State Electronics

journal homepage: www.elsevier.com/locate/sse

Graphene base heterojunction transistor: An explorative study on device potential, optimization, and base parasitics

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ARTICLE INFO

Article history:
Received 29 May 2015
Received in revised form 8 July 2015
Accepted 15 July 2015
Available online 28 July 2015

Keywords:
Base parasitics
Cut-off frequency
Graphene
Orientation
Simulation
Transistor

ABSTRACT

The Graphene-Base Heterojunction Transistor (GBHT) is a novel device concept with a high potential for analog high-frequency RF operation, in which the current is due to both thermionic emission and tunneling. In this paper we study through numerical simulations the influence of previously uninvestigated aspects of Si- and Ge-based GBHTs—namely, crystallographic orientation and doping density values—on the device performance; a comparison with an aggressively scaled HBT structure is then reported. The simulations are carried out with an in-house developed code based on a 1-D quantum transport model within the effective mass approximation and the assumptions of ballistic transport with non-parabolic corrections and ideal semiconductor–graphene interface. We show that crystallographic orientation has a negligible effect on the GBHT performance. The doping density values in the GBHT emitter and collector regions can be tailored to maximize the device performance: the Si device shows better overall performance than the Ge one, yielding a peak cut-off frequency f_T higher than 4 THz together with an intrinsic voltage gain above 10, or even higher f_T at the cost of a lower gain. The Si-based GBHT can potentially outperform the SiGe HBT by a 2.8 higher f_T. For a Si-based GBHT with a circular active region of diameter 50–100 nm, a theoretical balanced value for f_T and f_{max} above 2 THz can be achieved, provided the base parasitics are carefully minimized.

1. Introduction

In the last decade, graphene has gained a multifaceted attention from the scientific community. The potential offered by its 2-D nature [1], high-speed massless-like carriers, and group velocity in the range of 10^8 cm/s [2–5] have made it a serious candidate for enhancing the performance of RF devices. The demonstration of the graphene field-effect transistor (GFET) in 2004 [4] was the milestone that opened the way to the investigation of a variety of RF applications, including GFET-based integrated circuits [6,7], while GFETs themselves have reached current-gain cut-off frequencies above one hundred gigahertz [8,9]. In spite of this, challenges remain: the use of graphene in RF electronics is still limited by the absence of an energy gap and the reduced channel mobility due to extrinsic scattering sources [10], which are responsible for poor drain current saturation and limited cut-off frequency.

An alternative device concept was proposed by Mehr et al. [11], in which graphene forms the semimetallic base of a hot-electron tunneling transistor rather than the channel material. In this device, called graphene-base transistor (GBT), the current flows from the emitter to the collector region across the graphene layer [12], which, thanks to its monolayer thickness, should ensure a negligible base transit time—which represents one of the main contributions to the total transit time of the intrinsic transistor. However, in order to achieve top performance, the GBT requires a very low emitter Schottky barrier and a thin emitter-to-base tunneling layer: the lack of such features is one of the reasons for the poor performance of the first GBT prototypes [13,14].

In order to overcome the GBT limitations, in [15] we have investigated a new transistor architecture with graphene base, named graphene-base heterojunction transistor (GBHT). The GBHT is obtained by simply stacking an *n*-type semiconductor layer (emitter), a graphene monolayer (base), and another *n*-type semiconductor layer (collector). A qualitative schematic view is shown in Fig. 1. In terms of structure and behavior, it is similar to an *n*-*p*-*n* HBT, with the *p*-type base replaced with the graphene monolayer (which can be assumed undoped). A detailed simulation study by Schröter et al. [16] shows that cut-off frequency values above 1 THz can be achieved in SiGe HBTs through an

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http://dx.doi.org/10.1016/j.sse.2015.07.006
0038-1101/

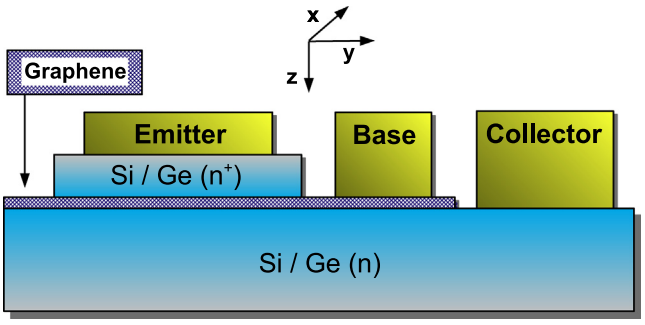

Fig. 1. Qualitative schematic view of the GBHT.

aggressive scaling: in principle, the removal of the base transit time thanks to a monolayer-thick graphene base layer shall push the GBHT to even higher operating frequencies.

GBHTs and GBTs share both the potential advantage represented by the minimized base transit time and the need for a high-quality, defect- and scattering-free graphene interface, a key factor on which the device performance strongly depends. However, the study of out-of-plane electron transport in graphene is still at an early stage, and goes beyond the scope of this paper, which therefore is focused on the intrinsic device, assuming an ideal graphene/semiconductor interface.

In our previous work [15], only ⟨100⟩-Si GBHTs were simulated: since in general the tunneling component of the device current is not negligible, it is recommendable to study all the main crystallographic orientations, characterized by different effective masses. Besides, silicon is not necessarily the best semiconductor choice for the emitter/collector layers, also considering the technological problems related with the graphene interface [17–19].

In this paper we study through numerical simulations the effect of crystal orientation on the performance of both silicon- and germanium-based GBHTs. We also show that a proper choice of both the emitter and collector doping density can boost the GBHT RF performance with a fair intrinsic voltage gain and an acceptable sensitivity with respect to the doping density variation. A comparison between a *n*-type Si GBHT and an optimized SiGe HBT structure is then carried out in order to estimate the potential advantage of the new device. The effect of the graphene base parasitics on the unity power gain frequency $f_{\max}$ of Si GBHTs is finally estimated, further extending the work carried out in [15].

The paper is organized as follows. In Section 2 the main features of the numerical model are summarized and the method for simulating any Si or Ge orientation is presented. In Section 3, the effect of the crystallographic orientation is discussed, followed by an optimization/sensitivity study based on the emitter and collector doping densities, together with a comparison between the two materials; a comparison between a n-Si GBHT and a SiGe HBT is then reported. In Section 4 the effect of the base parasitics on the device RF performance is studied. Finally, a conclusion is drawn is Section 5.

2. Numerical model and arbitrary orientations

The core of the numerical model adopted in this paper is the same already used in [15,12] for GBHT and GBT simulations, respectively. The model is one-dimensional: the device is assumed to be uniform in the x and y directions, so that $\vec{k}_t \equiv (k_x, k_y)$ is conserved, while transport occurs in the vertical z direction. Transport through the valence band is neglected. Electron transport is treated with the full-quantum ballistic approximation, within the non-equilibrium Green's function (NEGF) formalism [20], using for each conduction band valley an effective mass (EM) Hamiltonian with a non-parabolic effective mass correction derived from Flietner's energy-dispersion relation [21]

$$\epsilon(1+\alpha\epsilon) = \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z}\right), \tag{1}$$

with ϵ the electron kinetic energy, α the non-parabolicity factor, and $\hbar$ the reduced Planck constant. In this paper, $\alpha = 0.5\ \mathrm{eV}^{-1}$ is assumed for silicon [22], while the parabolic Hamiltonian is assumed for germanium ($\alpha = 0$).

We impose open-boundary conditions at the emitter and collector boundaries by defining appropriate self-energies, given by the closed-form expression reported in chapter eight of [20], valid for a semi-infinite lead. The graphene layer is assumed to be perfectly transparent to impinging electrons, as in [15], and hence the base current is neglected. Though optimistic, such assumption can be justified by the exploratory intent of this work. Very few aspects of carrier transport in the direction normal to graphene are known, and GBHT prototypes are still unavailable: for this reason we carry out a best-case study, focusing on the intrinsic device with ideal graphene interface (including base parasitics only), excluding effects like the lattice mismatch between the semiconductor and graphene (which might be one reason for the non-zero graphene reflectivity [23]), and the electron capture by graphene itself. The effect of graphene on the device electrostatics is fully taken into account by including in the 1-D Poisson equation the charge density on the graphene sheet calculated assuming the Dirac density-of-states model and the equilibrium occupation probability with Fermi energy equal to the base voltage. An equilibrium distribution with Fermi level equal to the base voltage is used in the semiconductor for holes too: in the absence of hole transport solving, this is the best approximation that can be taken, based on the p–n junction theory. The Poisson and the NEGF equations are solved self-consistently. The energy of the Dirac point E_D is set to $E_C(z_B) - \Phi_B$, with $E_C(z_B)$ the conduction band edge at the location of the graphene layer z_B and Φ_B the difference between the graphene workfunction and the electron affinity of the semiconductor: for silicon $\Phi_B = 0.5$ eV, for germanium $\Phi_B = 0.55$ eV.

The longitudinal and transverse effective masses are taken as $m_l = 0.92m_0$ and $m_t = 0.19m_0$ for silicon, $m_l = 1.6m_0$ and $m_t = 0.08m_0$ for germanium, respectively, with m_0 the free electron mass. In silicon for the ⟨100⟩ case (i.e., with the z-axis oriented along the ⟨100⟩ direction) the principal axes of the constant-energy ellipsoids are parallel to the reference axes x, y, z. Hence, for this orientation there are two families of subbands (ladders): the primed ladder with $m_x = m_y = m_t$, $m_z = m_l$ and degeneracy factor $g_v = 2$; the unprimed ladder with $m_x = m_z = m_t$, $m_y = m_l$ or $m_y = m_z = m_t$, $m_x = m_l$ and $g_v = 4$. For a general orientation, on the contrary, the EM tensor of the ellipsoids is not diagonal in the x, y, z reference. However, the following variable transformation can be applied to the retarded Green's function G^R

$$\widetilde{G^R}(z,z') = G^R(z,z')e^{\imath(z-z')\alpha}; \quad \alpha = \frac{w_{xz}k_x + w_{yz}k_y}{w_{zz}}, \tag{2}$$

where w_{ij} are the elements of the inverse EM tensor. Eq. (2) is the generalization to the NEGF formalism of the transformation proposed by Stern and Howard in [24] for the wavefunctions in the inversion layers of MOSFETs. This makes the Hamiltonian diagonal in the new reference system x_1, y_1, z, with the transverse coordinates x_1, y_1 rotated relative to the original ones x, y. The EM in the transport direction m_3 is equal to the inverse of w_{zz}, while the expressions of the transverse masses m_1 and m_2 are given by Eq. (13) of [24]. The values of such EMs for the Si and Ge orientations considered in this paper are reported in Table 1.