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Accurate Design of Si-Compatible Tunneling Field-Effect Transistor with GeSn Source Junction by *Ab Initio* Calculation and Device Simulation

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Abstract

In this work, *ab initio* calculation on GeSn, one of the advanced materials with high carrier mobilities and enhanced optical process probability, with various Sn fraction has been performed. The material parameters extracted from the first-principle simulation are fed into the device simulation in order to investigate the improvement of current drivability of tunneling field-effect transistor (TFET) having GeSn source junction in full consideration of bandgap tunability, effective mass, and effective density of states (DOS) of GeSn with different Sn fractions. It has been confirmed that the bandgap narrowing by Sn incorporation has predominance over the decrease of DOS so that current drivability is clearly reinforced. The atomic and device-level simulations are rigorously performed in strong cooperation to provide a technology for Si CMOS extension for low-power and high-speed applications.

1. Introduction

Tunneling field-effect transistors (TFETs) are low-power (LP) oriented owing to rather low current drivability when the device technology is realized by pure Si. Thus, although plausibly small subthreshold swing (S) and high on/off current ratio (I_{on}/I_{off}) are regarded as the merits of conventional TFETs, there remains to increase the current drivability for high-performance (HP), and relatedly, high-speed operations. I_{on} is effectively enhanced by introducing a narrow-bandgap material in the source junction and Ge can be a good candidate for its relatively small bandgap (0.66 eV) and superb Si compatibility [1]. GeSn is known to be an optical material due to its bandgap tunability and indirect-direct band transition capability by incorporating a proper amount of Sn [2,3]. In this work, new efforts to introduce GeSn to TFET technology are made. Further reduced energy-bandgap of GeSn would provide higher tunneling probability of valence electrons if the functional material is adopted to source junction. It is found from the *ab initio* calculation that effective density of states (DOS) is reduced as more Sn is incorporated [4]. Various parameters extracted from the electronic structures, including DOS, effective mass, optical and electrical energy bandgap (E_G) are fed into the device simulations to investigate the performances of GeSn-source TFET with a particular emphasis on its current drivability [5]. The Sn fractions are controlled 0, 5.55%, 8.33%, and 12.5%, and it is finally confirmed that the bandgap narrowing effect by higher Sn fraction is the dominant factor.

2. Characterization of GeSn by Atomic Simulation

The *ab initio* calculations of electronic structures of GeSn are primarily based on density functional theory (DFT). First, the lattice constants of GeSn with different Sn fractions were extracted from the volume optimizations by local density approximation (LDA) considering the exchange-correlated energy. The supercells had dimensions of 2×2×2, 2×2×3, and 3×3×2. For obtaining more realistic E_G values, modified Becke-Johnson (mBJ) model is coupled with LDA. Fig. 1 shows the accurate band structures along with the major material parameters.

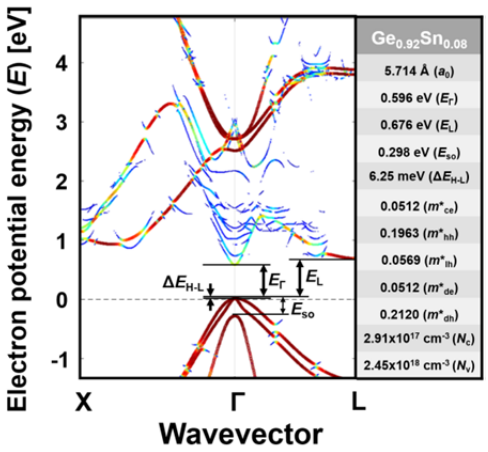

Fig. 1 *E-k* diagram and parameters of GeSn at 8.33% Sn.

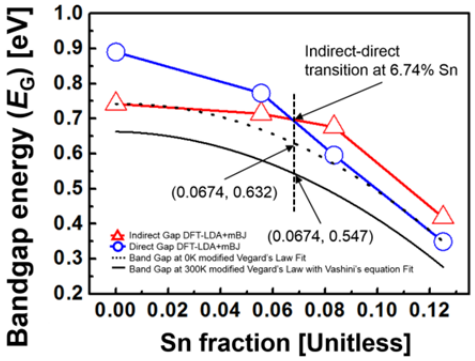

Fig. 2 E_G values as a function of Sn fraction and fitting.

For higher accuracy and credibility, temperature and Sn fraction dependences have been also considered to obtain the E_G's at room temperature by utilizing the modified Vegard's law (Eq. (1)) and Vashni's formula (Eq. (2)) simultaneously in cooperation.

$$E_{g0} = \frac{E_{g0}(\mathrm{Ge})}{0.125}(0.125 - x) + \frac{E_{g0}(\mathrm{Ge_{0.875}Sn_{0.125}})}{0.125}x - b(0.125 - x)x \quad (1)$$

(E_{g0}(Ge) = 0.742 eV, E_{g0}($Ge_{0.875}Sn_{0.125}$) = 0.349 eV, b = -26.23 eV)

$$E_g(\mathrm{Ge_{1-x}Sn_x}, T) = E_{g0} - \frac{10^{-4}\alpha T^2}{\beta + T} \quad (2)$$

Here, $\alpha = \exp(-37.48x^2 + 4.26x + 1.68)$ [eV/°C] and $\beta = -1066x^2 + 376x + 311$ [°C] (x: Sn fraction).

Further, the above equations are equipped with the empirical values in the existing literature [6]. The conductivity effective mass (m_c^*) and DOS effective mass (m_d^*) of electron were extracted by differentiating the minimum conduction valley in the ***k***-space contoured by different Sn fractions. Those of holes were obtained in the similar way and the heavy and light-hole band splitting was also considered [7]. m_c^* of electron is notably reduced as the indirect-to-direct bandgap transition takes place. At the same time, the electron m_d^* declines since the local minima valleys are sharpened. All the effects on bandgap narrowing, effective DOS in the valence band, effective masses are provided to device simulations.

3. Device Simulation for GeSn TFET Design

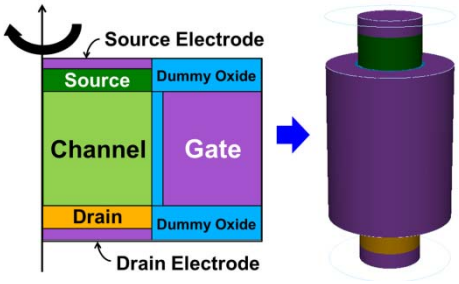

Fig. 3 Schematic of *n*-type TFET with GeSn/Ge/Si stack.

Fig. 3 shows the schematic of the designed *n*-type TFET having p^+ GeSn source/intrinsic Ge channel/n^+ Si drain stack. The above heterostructure can be schemed making a full use of high Si compatibility of Ge and the little lattice mismatch between Ge and GeSn. For introducing more models, 2-D structure is firstly constructed and made cylindrically symmetric for a 3-D structure. The channel length is fixed to 50 nm by which tunneling predominance and little dependence on channel mobility are expected [8]. By this approach, a more rigorous study on the effects of bandgap narrowing and DOS on current drivability by tunneling is made possible. The source doping concentrations are adjusted to the effective DOS in the valence band ($N_{v,eff}$) for fair comparisons: 6 × 10^{18} cm^{-3}, 3.08 × 10^{18} cm^{-3}, 2.45 × 10^{18} cm^{-3} and 2.19 × 10^{18} cm^{-3}, as Sn fraction changes 0, 5.55%, 8.33%, and 12.5%. Multiple models are included: band-to-band tunneling model by Hurkx, bandgap narrowing model universal to various semiconductor materials, Shockley-Read-Hall recombination model, Fermi-Dirac statistics, and non-local tunneling calculation. The material parameters obtained from the first-principle simulations are imported to the device simulations for highly reliable TFET characterization.

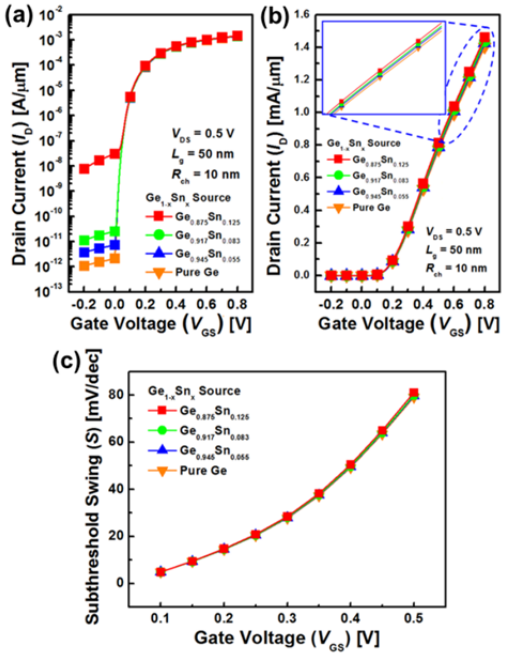

Fig. 4 Device performances. I_D-V_{GS} curves in the (a) logarithmic and (b) linear scales. (c) S vs. V_{GS}. V_{DS} = 0.5 V.

Fig. 4(a) shows the I_D-V_{GS} curves from the GeSn TFETs with different Sn fractions. Although $N_{v,eff}$ decreases as Sn increases and the valence electrons ready to tunnel into channel decrease, I_{on} increases since the bandgap narrowing effect is dominant, which is more clearly shown in Fig. 4(b). S depicts a monotonic increase with V_{GS} but the on-set S reaches down to sub-20-mV/dec as demonstrated in Fig. 4(c).

4. Conclusion

In this work, a rigorous study on Si-compatible heterojunction TFET having GeSn source junction is made through both atomic and device simulations. It is found that the radical bandgap tunability of GeSn has a merit in TFET operation despite of decrease in $N_{v,eff}$. GeSn TFET will be a plausible candidate for advanced electron device toward Si CMOS extension.

Acknowledgement

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References

[1] S. Cho *et al.*, Appl. Phys. Lett. **99** (2011) 243505.
[2] J. S. Harris *et al.*, ECS transactions **50** (2012) 601.
[3] S. Cho *et al.*, IEEE Photonics Technol. Lett. **23** (2011) 1535.
[4] *Wien2k Manual* online available at http://www.wien2k.at.
[5] *Atlas Users Manual* (Silvaco, Santa Clara, CA, 2015).
[6] K. Zelazna *et al.*, Jpn. J. Appl. Phys. **49** (2016) 235301.
[7] Q.-W. Kuang *et al.* Chin. Phys. B. **20** (2011) 127101.
[8] S. Cho *et al.*, IEICE Electron. Express **9** (2012) 828.