Atomistic analysis of band-to-band tunnelling in direct-gap $Ge_{1-x}Sn_x$ group-IV alloys

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***Abstract*—The emergence of a direct band gap in $Ge_{1-x}Sn_x$ alloys has stimulated interest in developing $Ge_{1-x}Sn_x$ alloys and nanostructures for applications in Si-compatible electronic and photonic devices. The direct band gap of $Ge_{1-x}Sn_x$, combined with the strong band gap reduction associated with Sn incorporation, makes $Ge_{1-x}Sn_x$ a promising material system for the development of Si-compatible tunnel field-effect transistors (TFETs) due to an expected strong increase in band-to-band tunnelling (BTBT). Based on a semi-empirical tight-binding model, we establish quantum kinetic BTBT current calculations for atomistic $Ge_{1-x}Sn_x$ alloy supercells. Recent analysis suggests that $Ge_{1-x}Sn_x$ possesses hybridised conduction band edge states for $x \lesssim 10\%$. We demonstrate that Sn-induced band mixing opens up a pathway for direct BTBT in ordered alloy supercells, strongly enhancing BTBT current compared to Ge. The framework we establish allows for quantitative prediction of the properties and performance of $Ge_{1-x}Sn_x$-based TFETs.**

I. Introduction

TFETs have the potential to overcome power dissipation issues related to channel size reduction in conventional complementary metal-oxide semiconductor (CMOS) FETs [1]. TFETs exploit BTBT to inject carriers into the device channel, with significant enhancements in performance predicted for TFETs utilising channels comprised of semiconducting thin films or nanowires. While Si and Ge are ubiquitous in conventional CMOS microelectronics, their indirect fundamental band gaps limit BTBT, which must rely on simultaneous phonon absorption/emission in order to conserve crystal momentum. Recently, group-IV alloys – primarily $Ge_{1-x}Sn_x$ – have emerged as a promising approach to realise CMOS-compatible direct-gap semiconductors, suitable for applications in electronic and photonic devices. The reduction in band gap with increasing Sn composition x in $Ge_{1-x}Sn_x$, combined with the emergence of a direct band gap in the composition range $6\% \lesssim x \lesssim 9\%$, make $Ge_{1-x}Sn_x$ alloys of particular interest for TFET applications [2], [3].

Emerging evidence indicates that $Ge_{1-x}Sn_x$ alloys possess a hybridised band gap for $x \lesssim 10\%$, with the alloy conduction band (CB) edge formed of an admixture of the Γ_{7c} and L_{6c} states of Ge [4], [5]. This Sn-induced band mixing suggests that the indirect- to direct-gap transition proceeds continuously with increasing x, via the transfer of Ge Γ_{7c} character to the alloy CB edge. This is in contrast to the assumption that a direct band gap emerges abruptly at a single, critical Sn composition, a conclusion incorporated a priori in calculations in which band mixing effects are neglected. From the perspective of TFET applications, the presence of a hybridised band gap in $Ge_{1-x}Sn_x$ can be expected to lead to the onset of appreciable *direct* BTBT at lower x, due to the acquisition by the alloy CB edge of an admixture of direct (Ge Γ_{7c}) character. To investigate this, we have established calculations of BTBT currents in $Ge_{1-x}Sn_x$ using an atomistic alloy supercell approach coupled to full-band quantum kinetic calculations. For ordered alloy supercells we demonstrate that pronounced Sn-induced band mixing opens up a pathway for direct BTBT in $Ge_{1-x}Sn_x$, strongly enhancing the BTBT current at fixed voltage compared to indirect-gap Ge.

II. Theoretical model

Our semi-empirical theoretical model encompasses a parametrised valence force field potential (VFF) and nearest-neighbour sp^3s^* tight-binding (TB) Hamiltonian, which are used respectively to compute the relaxed atomic positions and electronic structure of $Ge_{1-x}Sn_x$ alloy supercells. The VFF potential and TB Hamiltonian are parametrised using the structural, elastic and electronic properties – computed via density functional theory (DFT) – of the elemental diamond-structured materials Ge and α-Sn, and the IV-IV zinc blende compound GeSn. The accuracy of the VFF structural relaxations and TB electronic structure calculations for $Ge_{1-x}Sn_x$ alloy supercells has been verified via direct comparison to the results of DFT alloy supercell calculations [5]. Using the complex band structure calculated via the TB method, we compute BTBT current density as a function of applied voltage for [001]-oriented $Ge_{1-x}Sn_x$ nanowires – of total length 30 nm, constructed via supercell repeats along the [001] direction – using a non-equilibrium Green's function (NEGF) approach, as implemented in the OMEN software package [6]. To quantify the impact of Sn-induced band mixing effects on the BTBT current, we neglect electron-phonon coupling and restrict our attention here to the *direct* BTBT current.

III. Results

Figure 1(a) shows the calculated complex band structure of a pure 64-atom Ge_{64} supercell. In this $2 \times 2 \times 2$ simple cubic supercell, the lowest energy CB states at the supercell zone centre ($\mathbf{K} = 0$) are the folded L_{6c} CB edge states. We note that these states are *not* linked to the valence band (VB) edge states via a complex band, reflecting that there is no available path for *direct* BTBT from the Γ-point VB edge to the L-point CB minimum. The second lowest energy set of Ge_{64} CB states are the zone-centre Γ_{7c} states, which are linked via a complex band to the (light-hole-like) VB edge states. BTBT in Ge is then limited by (i) the indirect fundamental band gap, and (ii) the lowest energy CB states to which direct BTBT is possible lying ≈ 0.90 eV above the VB edge in energy. Correspondingly, we calculate a low BTBT current density

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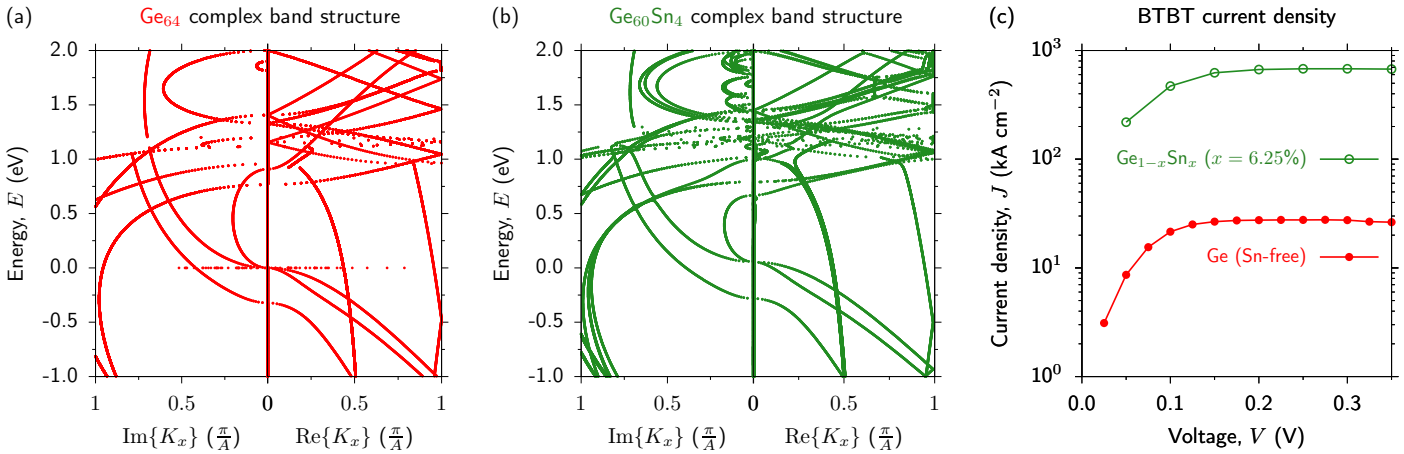

Fig. 1. Complex band structure of (a) a Sn-free Ge_{64} supercell, and (b) an ordered $Ge_{60}Sn_4$ ($x = 6.25\%$) alloy supercell. (c) BTBT current density as a function of applied voltage, for nanowires generated via Ge_{64} (closed red circles) and $Ge_{60}Sn_4$ (open green circles) supercell repeats along [001].

$J = 26$ kA cm^{-2} in a Ge_{64}-based nanowire for an applied voltage $V = 0.35$ V (closed red circles, Fig. 1(c)).

Next, we consider an ordered $Ge_{60}Sn_4$ ($x = 6.25\%$) alloy supercell, formed by substituting 4 Ge atoms in Ge_{64} by Sn on a face-centred cubic array. This supercell is equivalent to the ordered $Ge_{15}Sn_1$ ($x = 6.25\%$; $2 \times 2 \times 2$ face-centred cubic) supercell considered in Refs. [4] and [5], but allows for analysis of BTBT in an [001]-oriented nanowire. The L-point eigenstates in Ge_{64} fold to $\mathbf{K} = 0$, allowing for Sn-induced hybridisation between Ge Γ- and L-point states in $Ge_{60}Sn_4$. This results primarily in strong hybridisation between the Γ_{7c} and L_{6c} CB edge states of Ge, with the $Ge_{60}Sn_4$ alloy CB edge being formed predominantly of an admixture of Γ_{7c} and a linear combination of L_{6c} states possessing A_1 symmetry at Sn atomic sites [5]. The impact of this hybridisation is evidenced clearly in the complex band dispersion shown in Fig. 1(b), where we observe that this Sn-induced band mixing drives an anti-crossing between the complex bands originating from the Γ_{7c} and folded L_{6c} states of Ge. The result is the emergence of a complex band linking the aforementioned alloy CB edge state to the VB edge. In a simple, semi-classical description the BTBT transmission coefficient scales as an (inverse) exponential function of the area bounded by the complex band linking the CB and VB edges. The strong reduction in this area brought about by a combination of Sn-induced band gap reduction and CB edge hybridisation is therefore expected to lead to a strong increase in BTBT current density at fixed voltage compared to Ge. Indeed, for a $Ge_{60}Sn_4$-based nanowire we calculate $J = 0.67$ MA cm^{-2} for $V = 0.35$ V, which is ≈ 25 times larger than that calculated for the Ge_{64}-based nanowire at the same voltage (open green circles, Fig. 1(c)).

IV. Conclusion

We have undertaken a theoretical analysis of direct BTBT in $Ge_{1-x}Sn_x$ alloys, using an atomistic alloy supercell approach. Our ordered supercell calculations highlight that Sn-induced hybridisation plays an important role in determining the nature of BTBT in $Ge_{1-x}Sn_x$ alloys: the hybridised nature of the $Ge_{1-x}Sn_x$ alloy CB edge – comprised of an admixture of the Γ_{7c} and L_{6c} states of Ge – enhances direct BTBT at Sn compositions below which the indirect- to direct-gap transition is generally assumed to occur. This, combined with the strong Sn-induced band gap reduction, contributes to strongly enhanced BTBT current compared to Ge. Our results reaffirm the potential of $Ge_{1-x}Sn_x$ alloys for TFET applications. However, the importance of band mixing effects is likely to be overestimated in small, ordered supercell calculations compared to realistic, disordered alloys. The framework we have established to investigate BTBT in $Ge_{1-x}Sn_x$ alloys is highly scalable, allowing for application to large-scale atomistic simulations of realistic $Ge_{1-x}Sn_x$ alloy thin films and nanowires, and hence to quantify the impact of alloy disorder effects on BTBT current and associated implications for TFET applications.

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References

[1] A. M. Ionescu and H. Riel, "Tunnel field-effect transistors as energy-efficient electronic switches," *Nature*, vol. 479, p. 329, 2011.

[2] S. Sant and A. Schenk, "Band-offset engineering for GeSn-SiGeSn hetero tunnel FETs and the role of strain," *IEEE J. Electron. Devi.*, vol. 3, p. 164, 2015.

[3] E. Galluccio, J. Doherty, S. Biswas, J. D. Holmes, and R. Duffy, "Field-effect transistor figures of merit for VLS-grown $Ge_{1-x}Sn_x$ ($x = 0.03$-0.09) nanowire devices," *ACS Appl. Electron. Mater., in press*, 2020.

[4] T. D. Eales, I. P. Marko, S. Schulz, E. J. O'Halloran, S. Ghetmiri, W. Du, Y. Zhou, S.-Q. Yu, J. Margetis, J. Tolle, E. P. O'Reilly, and S. J. Sweeney, "$Ge_{1-x}Sn_x$ alloys: consequences of band mixing effects for the evolution of the band gap Γ-character with Sn concentration," *Sci. Rep.*, vol. 9, p. 14077, 2019.

[5] E. J. O'Halloran, C. A. Broderick, D. S. P. Tanner, S. Schulz, and E. P. O'Reilly, "Comparison of first principles and semi-empirical models of the structural and electronic properties of $Ge_{1-x}Sn_x$ alloys," *Opt. Quant. Electron.*, vol. 51, p. 314, 2019.

[6] M. Luisier and G. Klimeck, "OMEN: an atomistic and full-band quantum transport simulator for post-CMOS nanodevices," *Proc. 8th IEEE International Conference on Nanoelectronics*, 2008.