

Framework for Investigating Cryogenic Hole Mobility in Group-IV-Alloy Quantum Wells

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Abstract—This work presents a comprehensive three-stage framework for investigating the electrical properties of quantum well heterostructures fabricated in the group-IV alloy system. It begins with first-principles calculations via density functional theory to extract key material properties. This is followed by a self-consistent solution to the Schrödinger-Poisson system to obtain electrostatic properties of carriers under quantum confinement. The last step solves the Boltzmann transport equation using the ensemble Monte-Carlo method. The simulation results are validated with experimentally measured values, demonstrating the capability of the solver.

Index Terms—Modeling and simulation, density functional theory, GeSn, bandstructure, hole mobility.

I. INTRODUCTION

The bandstructure of Ge-rich group IV alloys can be engineered to obtain a direct energy bandgap, alongside high carrier mobilities. This presents the prospect of mimicking II-VI and III-V semiconductors using an all group IV alloy system (SiGe, GeSn, SiGeSn, SiSn), and thus the possibility of monolithic integration of electronics and photonics. Furthermore, group IV alloys show potential for a wide range of applications like thermoelectrics, quantum optics, quantum dot arrays, etc [1]. As such, a thorough understanding of their electrical properties is needed to exploit the full potential of this material system. Ge-rich quantum wells are particularly interesting for a variety of applications that require high hole mobilities. Similar to high electron mobility in Si-rich Si/SiGe quantum wells (QWs) [2], [3], Ge-rich GeSn quantum wells have demonstrated hole mobilities of the order of $10^6 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ [1], [4]. It is well known that inclusion of mechanical strain can be used to engineer electronic band structure, while simultaneously enhancing hole mobility in

Ge. The bandstructure can further be modified by alloying with Sn [5], [6], and the possible existence of short-range order (SRO) [7], [8]. Alloying Ge with heavy metals like Sn and Pb also leads to strong spin-orbit coupling (SOC) [9]. The hole transport in alloyed Ge QWs is further influenced by operating temperatures and applied bias. Consequently, in order to understand the electrical properties of this material system, we need a comprehensive model that can include and investigate the effect of these material properties.

In this study, we present a computational framework that investigates electrical transport by solving the Boltzmann transport equation (BTE) using a particle-based simulation method, supported by first-principles calculations using density functional theory (DFT). The simulation framework is validated with experimentally observed hole densities and mobilities in Ge-rich GeSn QWs [10].

II. METHODOLOGY

A complete solution of carrier transport requires solving a many-body Schrödinger equation, which is nearly infeasible, even with modern-day computing power. Thus, we use the ensemble Monte-Carlo (MC) method to calculate a path integral solution to the BTE [11]. This is a particle-based simulation method, and such a method requires an a priori knowledge of certain material parameters like effective mass, deformation potentials, electron bandstructures, etc. These are generally known for conventional materials like Si, Ge, GaAs, GaN, etc., but need to be ascertained for GeSn alloys. In this work, we obtain relevant GeSn parameters via DFT calculations. The physical geometry of the QW heterostructures leads to the formation of a quasi-two-dimensional hole gas (Q2DHG) due to quantum confinement. The carriers are confined in the direction perpendicular to the GeSn/Ge hetero-interface, and are free to move in the in-plane directions. This Q2DHG

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further complicates the simulations by imposing restrictions on carrier distributions. These need to be resolved by solving a self-consistent Schrödinger-Poisson (SCSP) problem [12]. Thereafter, we use a two-dimensional Monte Carlo (2DMC) solver, which calculates the low-field transport properties of the material system of interest. The complete framework is thus divided into three parts: (1) DFT, (2) SCSP, and (3) 2DMC solution of BTE.

The DFT calculations are performed using Vienna ab-initio simulation package (VASP) [13] based on the projection augmented wave method [14]–[16]. We use a special quasi-random structure (SQS) [17] to represent the $\text{Ge}_{1-x}\text{Sn}_x$ solid solution. These are performed by utilizing the modified Becke-Johnson exchange potentials (mBJ) in combination with local density approximation (LDA) correlations. It also includes the effect of SOC.

The solution of the SCSP system at low temperatures is a numerically challenging problem due to the highly non-linear nature of the Poisson equation. We employ higher-order numerical schemes to ensure consistent convergence to real, physical solutions. This includes solutions with the finite volume method (FVM) [18], [19], using 9-point Chebyshev-Curtis quadrature approximation for the integrals. The resulting system of linear equations is solved using the Newton-Raphson method. The results of the SCSP include information about carrier electrostatics. It provides population, eigenenergies, and eigenvectors (wavefunctions) of the quantized subbands along with conduction and valence band profiles.

This information is then used in the 2DMC module to simulate carrier transport. Under the influence of an external electric field, which is applied in the direction parallel to the GeSn/Ge interface, carriers follow a free-flight-scatter trajectory. Carriers experience scattering due to various physical phenomena like phonon interaction, Coulomb centers, surface roughness, etc [11]. These are characterized by their respective perturbation potentials and evaluated using Fermi's Golden rule [20]. The model incorporates all possible inter- and intra-band and inter- and intra-subband scattering mechanisms. To calculate the scattering rates, we follow the formalism presented in [1], [21]. For GeSn QW of interest, important scattering mechanisms are acoustic phonon, non-polar optical phonon, alloy disorder, and surface roughness scattering. The 2DMC simulations are run for an ensemble size of 10^6 particles to reduce statistical noise.

III. RESULTS AND DISCUSSION

The framework is validated for the device shown in Fig. 1. It is a 10 nm, strained GeSn (with 9% Sn) layer sandwiched between two Ge layers. The concentration profiles extracted via secondary ion mass spectrometry (SIMS) show a graded (1.51% nm^{-1}) junction between Ge and GeSn layers. The device is nominally undoped with a background impurity density of $1 \times 10^{15} \text{ cm}^{-3}$ [10]. The study is performed to understand the behavior of the device at cryogenic temperatures (between 4K and 20K).

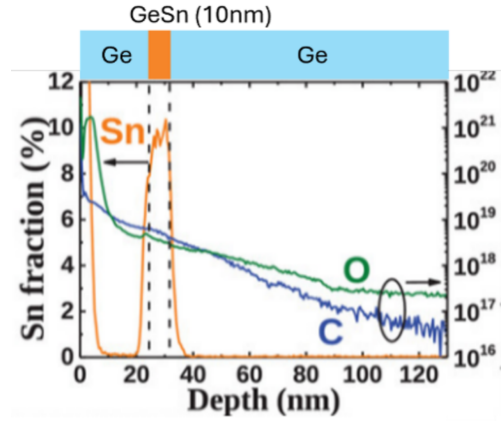


Fig. 1. The structure studied in this work [10]. The compositional variation of Sn (orange line) shows a sharp, but graded QW junction.

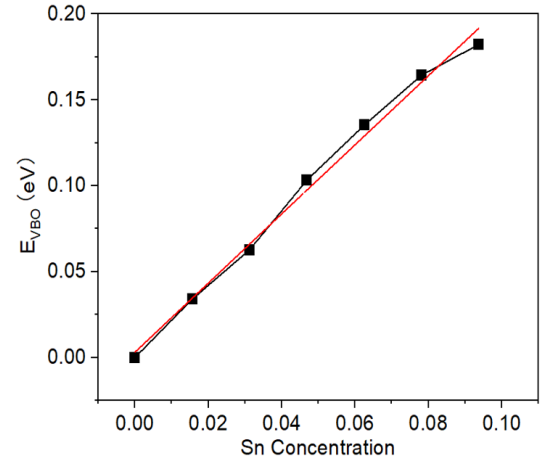


Fig. 2. Variation of the valence band offset at the Ge/GeSn hetero interface for different Sn concentrations (x). The red curve is the extracted empirical relation valid for small x ($<10\%$). The black curve shows DFT calculations.

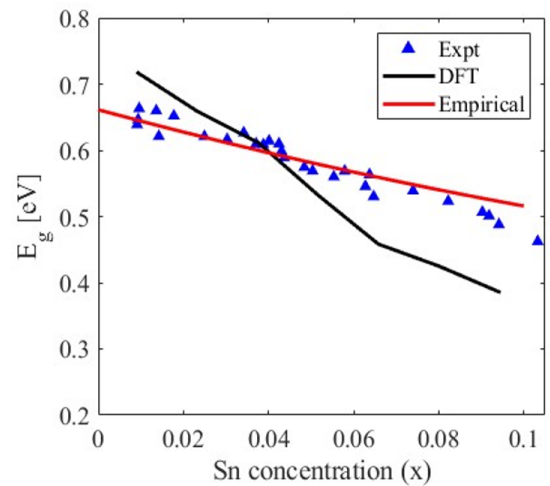


Fig. 3. Experimental [22] and DFT GeSn bandgaps. The empirical model is fit to experimentally measured E_g because DFT is known to underestimate bandgaps at high Sn concentrations.

The valence band offsets (VBO), and energy bandgaps (E_g) computed via the DFT framework are presented in Figs. 2 and 3 respectively. They are fit to empirical relations to reduce computational burden. The concentration (x) dependent VBO and E_g are given below,

$$\text{VBO(eV)} = 2.01x + 3.75 \times 10^{-3} \quad (1)$$

$$E_g = 0.742 - \frac{4.8 \times 10^{-4} T^2}{T + 235} - 1.74x + 2.86x^2 \quad (2)$$

The electron bandstructures for relaxed Ge and relaxed GeSn (x=8%) along the $L \rightarrow \Gamma \rightarrow X \rightarrow K \rightarrow \Gamma$ are shown in Fig 4(a) and (b) respectively. The bandstructure of compressively strained GeSn near the VBM is shown in Fig 4(c). Alloying and strain lead to the splitting of HH and LH bands. As a result, it is no longer accurate to call them HH, LH, and SO bands in a traditional sense, as they do not necessarily correspond to heavier or lighter hole effective masses. Hereafter, we refer to them as valence bands 1, 2, etc. (VB1, VB2, etc.). It is important to note that the Brillouin zone of the supercell is smaller than the primitive cell, and band folding does not alter the curvature around the Γ -point, enabling accurate extraction of hole effective masses. The extracted masses show anisotropic behavior, which is correctly accounted for in our framework. It is demonstrated that the effective masses obtained this way match experimentally measured effective masses [1].

The carrier wavefunctions of the lowest two subbands and the valence band edge are shown in Fig. 5, clearly showing effects of carrier confinement. It is observed that the subbands corresponding to valence bands VB2 and VB3 are substantially less populated due to the energy offset from the VBM. This is further exacerbated at low temperatures, where carriers have less thermal energy and occupy low-energy subbands. As the gate bias is increased, the top Ge layer is pulled up, leading to the formation of a parallel channel at the top oxide-Ge interface. In this study, we discuss the regime of low applied bias where a single channel is present (and confined) in the GeSn QW region. The framework can be expanded to simulate regimes of high applied bias wherein two parallel channels contribute to electrical transport [1].

The low temperature hole mobility vs. sheet carrier density is shown in Fig. 6. We observe good agreement with the experimentally measured values (<5%). At low temperatures, small phonon populations lead to negligible phonon-based scattering (acoustic and non-polar optical phonons). Consequently, the hole mobility is limited by alloy disorder and surface roughness scattering mechanisms. Out of these, surface roughness scattering plays a dominant role under high gate bias, under which a parallel channel is formed at the oxide-Ge interface. The alloy disorder scattering itself is dependent on the alloy disorder scattering potential (ΔU). In a random alloy, the difference in the atomic potentials of constituent atoms leads to a non-uniform potential surface. This leads to the rise of alloy disorder scattering [23], and ΔU captures the strength of this scattering mechanism. Some methods to estimate ΔU

include atomistic tight binding [24], DFT [25] calculations. In this study, ΔU is obtained via DFT calculations with some additional corrections. The most accurate way to determine the alloy disorder scattering potential for alloys (solid solutions) is still an unanswered question for the scientific community.

IV. CONCLUSION

The framework is generalized to study electrostatics and low-field electrical transport for different material combinations, and an arbitrary number of layers grown along arbitrary crystallographic directions. The study shows the effect of alloying and strain on GeSn bandstructures. We also present empirical relations for GeSn energy bandgaps and Ge/GeSn valence band offsets. The carrier electrostatics are computed via the SCSP module to effectively capture the impact of carrier confinement. Ultimately, the simulated 2DMC gives hole mobility values that agree with experimental measurements.

The results presented here demonstrate the capability of the framework to accurately estimate and explain hole mobilities. Furthermore, they also emphasize the contribution and the need of all constituent modules (DFT, SCSP, and 2DMC) to capture and explain the physics of GeSn QW devices at cryogenic temperatures. We also identify mobility-limiting mechanisms under different operating conditions. Simulation at cryogenic temperatures is of increasing interest in the scientific community today because of its relevance to the field of quantum computing.

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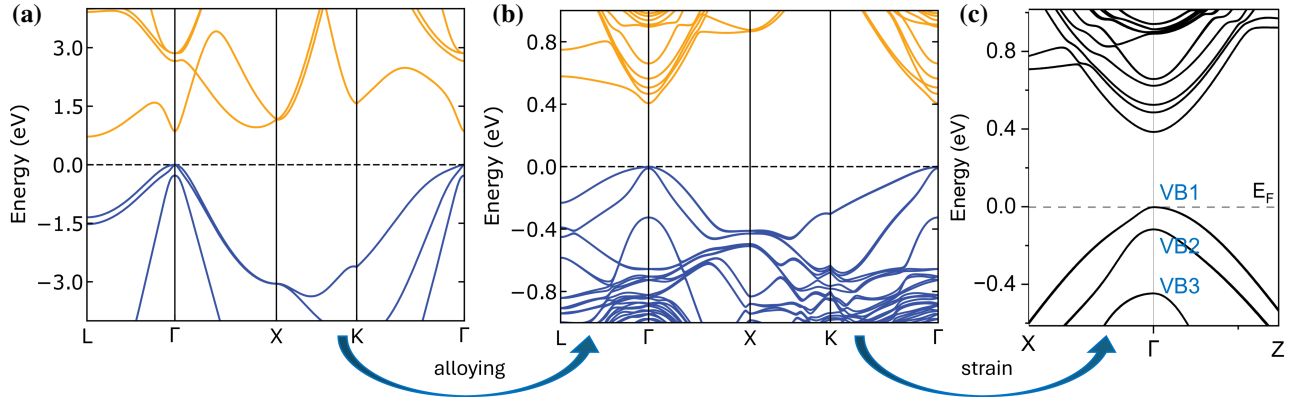


Fig. 4. Band structure of (a) relaxed Ge, (b) relaxed GeSn ($x=8\%$), and (c) GeSn under biaxial compressive strain. The effect of alloying and strain that leads to the splitting of heavy-hole (HH), and light-hole (LH) bands at the Γ point is shown in (c).

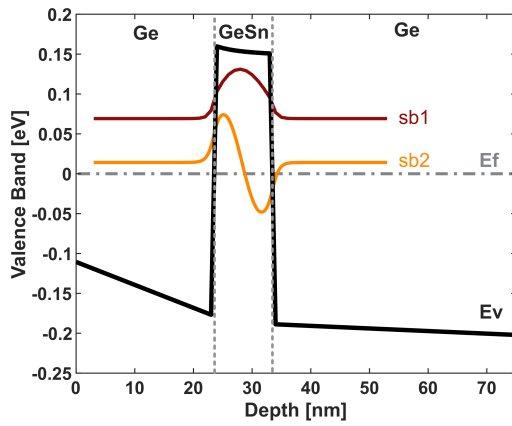


Fig. 5. Valence band profile (shown in black) and carrier wavefunctions (color) obtained by solving the SCSP problem at 1.2 K. We show the behavior only of the lowest two subbands that can be populated at cryogenic temperatures. Sb1 = subband 1, sb2 = subband 2, Ef = Fermi energy (reference), Ev = valence band maximum.

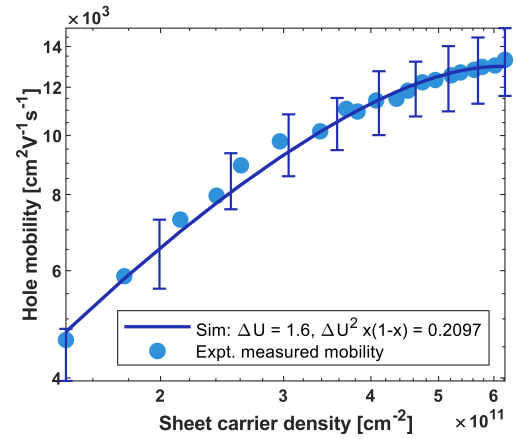


Fig. 6. Hole mobility vs. sheet carrier density at 1.2 K. The solid line represents simulated mobility values along with the corresponding 95% confidence intervals. The intervals represent a range of possible hole mobility values inclusive of experimental errors. Solid circles represent hole mobility values measured via Hall bar measurements.

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