Modeling Electrostatics and Hole Transport in (Si)GeSn Heterostructures

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***Abstract*—The demonstration of device-quality epilayers and quantum-engineered heterostructures fabricated in (Si)GeSn materials highlights the possibility of tunable all-group IV Si- integrated electronics and infrared photonics. This work introduces a comprehensive simulation framework that allows one to calculate the electrostatics and the transport characteristics of arbitrary (Si)GeSn heterostructures for a wide range of temperatures. The simulated results show excellent agreement with experimentally measured data, thus validating the capability of the solver.**

Keywords—(Si)GeSn Alloys, Heterostructures, Hole Mobility, Schrödinger-Poisson Solver, Ensemble Monte Carlo Method

I. Introduction

(Si)GeSn alloys constitute isovalent substitution of group-IV elements in cubic diamond-structured (Si)Ge lattices. This emerging family of semiconductors provides strain and composition as two degrees of freedom to independently engineer lattice parameters and the band structure [1,2]. For example, the tensile strain boosts the electron mobility of Ge material by a factor of two, whereas compressive strain leads to higher hole mobilities [3]. The substitution of Sn into Ge lattice to form the semiconducting $Ge_{1-x}Sn_x$ alloy is another possible route for tuning the electronic properties of Ge. The small energy separation of 140 meV between the indirect (L) and direct (Γ) conduction band valleys in Ge can be overcome by alloying with Sn as shown schematically in Fig. 1 [4], thus paving the path for achieving efficient light emission. The prospects of mimicking III–V and II–VI heterostructures and devices using all-group IV semiconductors on a Si platform have garnered significant interest, being motivated by the potential to achieve monolithic integration of electronics and photonics [5].

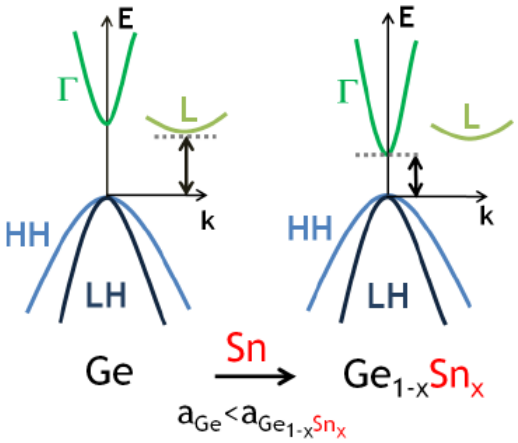

Fig. 1. Schematic showing the effect of Sn alloying on the band structure of Ge [4].

It has also been suggested theoretically that the (Si)GeSn material system might exhibit short-range order [6,7], which can serve as an additional degree of freedom for designing devices. Short-range chemical order (SRO) has been shown to play a decisive role in modulating a wide range of physical properties in medium-entropy alloys and high-entropy alloys. The enormous configurational space of these alloys implies multiple forms of SRO may exist. Such co-existence of SROs suggests an inherent structural heterogeneity, a diffuse electronic structure, and a new route for band engineering in Si–Ge–Sn medium-entropy alloys [8].

Based on the above discussion, it is evident that there is a need to develop a simulation framework that can accurately model the transport properties of these novel materials and the devices fabricated in the (Si)GeSn material system. To be able to accurately study the transport properties of holes in a variety of (Si)GeSn heterostructures, we have developed a comprehensive simulation framework that uses density functional theory results as input parameters into a 1D self-consistent Schrödinger-Poisson (SP) solver [9]. The outputs of the SP solver (subband population, wavefunctions and corresponding eigen-energies) are then fed into a Quasi-Two-Dimensional Monte Carlo (Q2DMC) solver that solves the Boltzmann Transport Equation (BTE), to obtain the low-field hole mobilities [10]. We use Q2DMC solver as this simulator allows us to investigate not only the low-field mobilities but also allows us to study the high-field transport characteristics of both electrons and holes in these heterostructures. Furthermore, the existing Q2DMC solver can be coupled to a 2D or 3D Poisson solver [11] to study possible (Si)GeSn device characteristics.

The paper is organized as follows: In Section II we describe the main features of our SP solver coupled to the Q2DMC. Section III presents a comparison of the simulation and the experimental (Hall measurement) temperature-dependent hole mobility data. Conclusions related to this study and prospects for devices fabricated using this material system are discussed in Section IV.

II. Simuulator Description

To be able to calculate the subband structure and study transport characteristics of holes in these (Si)GeSn heterostructures, it is necessary to calculate the effective masses of the heavy-hole, light hole and the split-off bands. First-principles density functional theory (DFT) calculations, that utilize the Vienna *ab initio* simulation package (VASP), are performed for this purpose and are based on the projector augmented wave method [12]. The Special Quasi-random Structure (SQS) method is used to represent the GeSn random solid solution with a simulation cell containing 128 atoms, obtained by replicating a primitive diamond cubic cell four

times along each dimension [13,14]. For this purpose the mcsqs code is utilized as implemented in the Alloy Theoretic Automated Toolkit (ATAT) package. A similar model of local density approximation (LDA) and modified Becke and Johnson (mBJ) method [15] was used to calculate the valence band maxima (VBM) offset between the $Ge_{1-x}Sn_x$ (x = 0.08) and the Ge layers in the heterostructure of interest using VASP. The VBM offset between $Ge_{1-x}Sn_x$ alloy and Ge is obtained employing the method proposed by Van de Walle for biaxially compressed $Ge_{1-x}Sn_x$ layer [16]. Simulation results for the electronic structure and the valence band offsets are shown in Fig. 2.

As shown in the flow-chart from Fig. 3, the extracted anisotropic effective mass tensors, valence band offsets and the energy bandgaps are fed into the self-consistent SP solver. Note that the solution of the SP system of equations at low temperature is a challenging task. The system matrix generated by the discretization of the Poisson equation has a large condition number, making it extremely difficult to solve using conventional numerical methods. We implement a scheme based on the 1st order Finite Element Method (FEM) with a high-order integration scheme (Chebyshev quadrature of the 9th order) to circumvent this problem [9]. When studying transport at low temperatures, partial ionization of the dopants must be accounted for.

Having calculated the subband structure and the population of carriers amongst various subbands, the next step in the simulation procedure is the calculation of the temperature dependence of the hole mobility in the quasi-2D confined system. The Monte Carlo method adopted for quasi-two-dimensional hole gas (Q2DHG) is used for the solution of the BTE. Relevant scattering mechanism incorporated in our theoretical model include acoustic phonon, non-polar optical phonon, and alloy disorder scattering [17]. At present, Coulomb scattering and screening of the scattering potentials is not accounted for. Note that in order to correctly account for screening of the acoustic phonons scattering potential, it is necessary to use dynamical screening. Since this is a very formidable task, it is 'less wrong' to keep the acoustic phonon scattering potential unscreened [18].

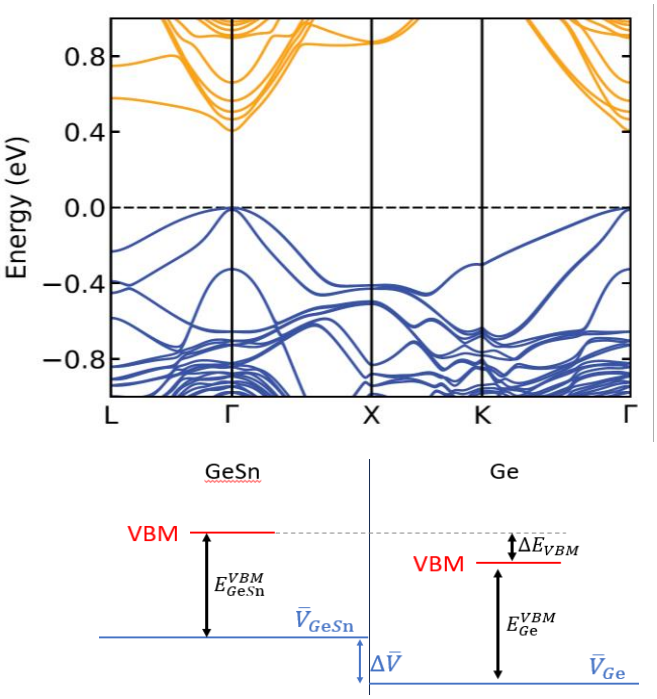

Fig. 2. Top panel: Folded electronic band structure of $Ge_{1-x}Sn_x$ alloy calculated using 128-atom SQS supercell with DFT. Bottom panel: calculated valence band offsets. For x = 0.08, ΔV =183±7 meV

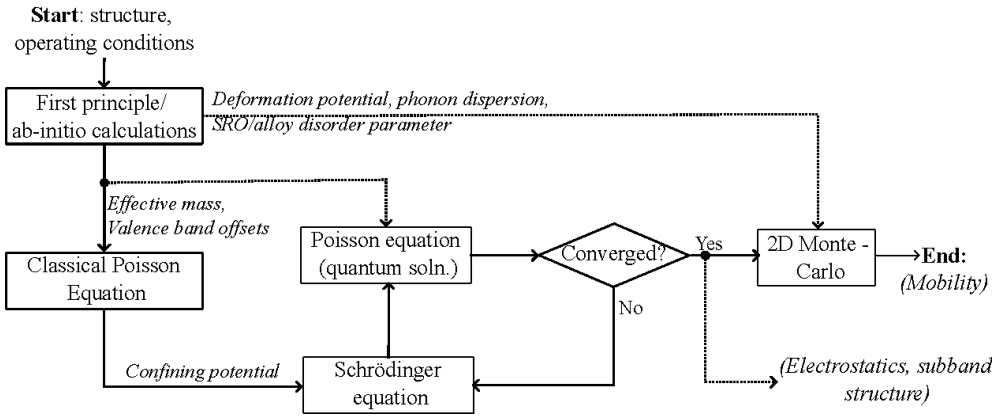

Figure 3. Flowchart explaining the hierarchical framework

The Q2DMC utilizes a free-flight-scatter scheme [19,20,21,22], wherein the carrier scattering rates are calculated within the first-Born approximation that utilizes Fermi's Golden Rule [23]. When calculating the scattering rates, we account for both intra-subband and inter-subband transitions (the inter-subband transitions can be within a given band or between different bands). The strength of these transitions depends upon the magnitude of the overlap integrals. Note that the acoustic and non-polar optical phonon vibrations are considered within the bulk phonon approximation.

The matrix element squared for scattering between subbands *n* and *m* due to acoustic phonons is of the form [24]:

$$\left|\left\langle n\left|U^{ac}(\mathbf{q})\right|m\right\rangle\right|^2 = \frac{k_B T}{\rho V v_s^2}\Xi^2 F_{nm}, \qquad (1)$$

where the form factor F_{nm} is calculated using:

$$F_{nm} = \int_0^\infty \left|\psi_n(z)\right|^2 \left|\psi_m(z)\right|^2 dz \qquad (2)$$

Ξ is the acoustic phonon deformation potential derived from first principles calculations, V is the volume and v_s is the sound velocity. The matrix element squared for non-polar optical phonon scattering is given by:

$$\left|\left\langle n\left|U^{op}(\mathbf{q})\right|m\right\rangle\right|^2 = \frac{\hbar D_o^2}{2\rho V \omega_o} F_{nm}, \quad (3)$$

where D_o is the non-polar optical phonons deformation potential and ω_o is the phonon frequency.

When calculating the alloy disorder scattering potential we use virtual crystal approximation that leads to the following expression for the matrix element squared for scattering between subbands n and m:

$$\left|\left\langle n\left|U^{alloy}(\mathbf{q})\right|m\right\rangle\right|^2 = \frac{x(1-x)a_0^3}{8V}\Delta V_{alloy}^2 F_{nm}, \quad (4)$$

where ΔV_{alloy} is the alloy disorder scattering potential and a_o is the lattice constant.

III. Simulation Results

Our in-house self-consistent SP solver functionality was tested on a simple heterostructure with a GeSn (8% Sn) layer grown on a Ge substrate (Fig. 4). The compressively strained SiGe layer is considered as a random alloy [9]. The study investigates three different samples labelled as 'low', 'medium', and 'high', indicating respective doping concentrations. Fig. 4 depicts the structure and the corresponding doping profiles. Experimental sheet carrier densities and mobilities are derived from Hall measurement technique at Sandia National Lab. In previous work [9] we have validated the SP solver by comparing the temperature dependence of the experimental sheet carrier densities with our simulation results. At lower temperatures, incorporation of the partial ionization of dopants was necessary to explain the experimental data.

In Fig. 5 we show a comparison between the simulated and the experimentally measured hole mobilities for the sample with 'low' doping. The deviation of simulations from experimental data for temperatures below 50K is explained by the absence of impurity (Coulomb) scattering from the model, which dominates at low temperatures. The non-uniform dopant concentration (as seen in Fig. 4), necessitates a real space treatment of the ionized impurities scattering. This is beyond the capability of the current solver, but the authors are expanding on it to accurately simulate Coulomb scattering for non-uniform doping profiles. Nevertheless, the agreement is excellent for temperatures larger than 50 K in which range alloy disorder and phonon scattering dominate.

The scattering potential for alloy disorder scattering needed to match the experimental data equals 1.2 eV. This is very close to values published in the literature for bulk SiGe random alloys as a reference [25,26]. Future studies within our group will focus on derivation of the allow disorder scattering potential from first principles. This can give a better insight on the importance of alloy disorder scattering mechanism in samples in which it is believed and it is experimentally determined whether short-range order exists.

IV. Conclusions

In summary, a simulation hierarchy was presented that combines DFT calculations for the electronic structure, the effective mass 1D self-consistent SP solver, and an effective mass Q2D Monte Carlo solver for the calculation of the temperature dependence of the hole mobility. This simulation framework allows us to explain quite closely the trend in the experimental data. We find that acoustic phonon scattering starts to be important at temperatures higher than 100 K. The alloy disorder scattering potential, which at present is considered as a fitting parameter, gives us information on the strength of this scattering mechanism for the case of a random alloy. Present studies are directed towards understanding of the role of short-range order in heterostructures with record high mobilities, having as a reference the value of the alloy disorder scattering potential for a GeSn random alloy used in this work.

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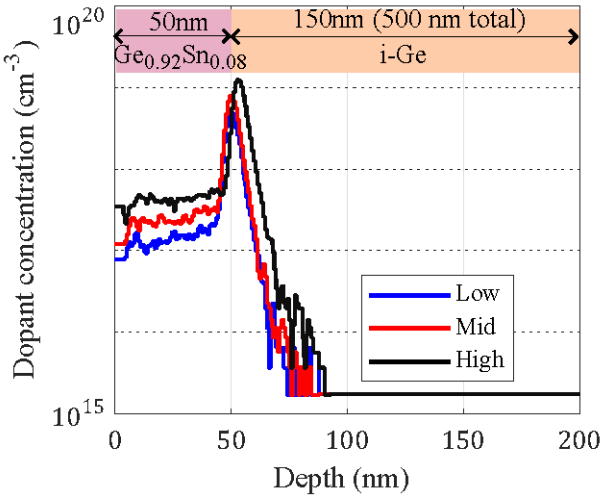

Fig. 4. Doping profiles for the three structures labeled as having 'low', 'medium' and 'high' doping. The structure being simulated is shown in the inset. SIMS measurement technique was used to extract the doping profiles of the three samples being considered in our studies.

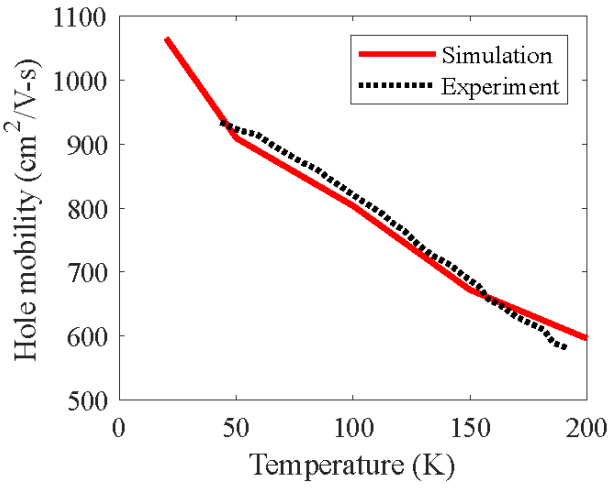

Fig. 5. Comparison of the simulated (solid line) and the experimental (dotted line) Hall hole mobility at different temperatures. Shown here is a comparison with experiments for the 'low' doped sample in which Coulomb scattering, except at very low temperatures, does not play significant role. For the samples having 'medium' and 'high' doping, it will be necessary to include Coulomb scattering and screening of this scattering potential.

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