

# Alloy-scattering-limited Hole Mobility in SiGe: First-principles-based Multi-scale Approach

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**Abstract**—In this work, we present a first-principles based multi-scale framework for calculating alloy-scattering-limited hole mobility in SiGe. In order to bridge between density functional theory (DFT)-based atomistic calculations and k.p based continuum model for multi-scale calculations, we have developed the absolute potential model. This model accurately reproduces the DFT based non-equilibrium green's function (NEGF) transmission results while improving computational efficiency by orders of magnitude. The calculated mobility for various compositions is consistent with experimental data.

**Index Terms**—SiGe, Hole mobility, DFT, First-principles, Alloy-scattering, NEGF

## I. INTRODUCTION

SiGe has attracted considerable attention as a promising channel material for advanced p-type field-effect transistors because of its favorable hole transport properties, tunable band structure through Ge composition, and compatibility with Si-based technology [1], [2]. However, since SiGe is an alloy, random atomic-scale disorder is inherently present and can significantly influence carrier transport [3]. In this context, accurate evaluation of alloy-scattering-limited hole mobility is essential for reliable transport analysis.

Previous studies have employed atomistic tight-binding approaches combined with Fermi's golden rule and Kubo–Greenwood formalism to analyze alloy-scattering-limited hole mobility in SiGe [4], [5]. While such methods provided useful physical insight, their predictive capability is limited by the empirical nature of parameterization and the approximations involved in describing scattering and transport.

To overcome the limitations of existing approaches, we perform computationally demanding, parameter-free first-principles calculations of alloy-scattering limited hole mobility in SiGe by statistically sampling many random-alloy configurations that are realized at the atomistic scale by DFT. To extend such calculations and make them tractable for device-level simulations, we also develop a computationally efficient absolute potential model that accurately reproduces the DFT-based transport results.

## II. DFT CALCULATION

For the rigorous evaluation of alloy-scattering in SiGe, the DFT-based non-equilibrium Green's function (NEGF) workflow is employed [6]. As illustrated in Fig. 1, we first construct

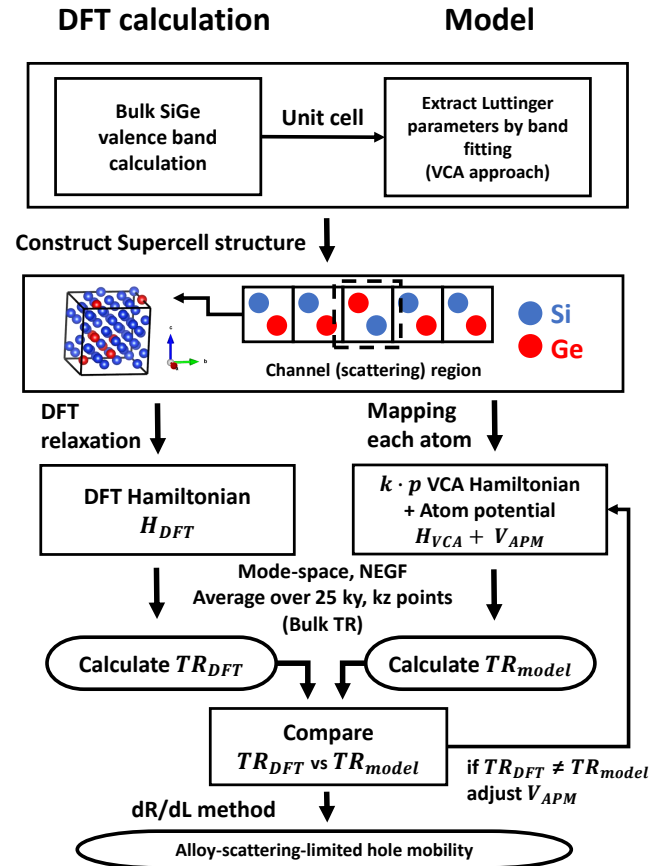


Fig. 1. Overall workflow of the simulation to calculate alloy-scattering-limited hole mobility in SiGe

a cubic unit cell containing 64 atoms. The coordinate axes are defined as  $x \parallel [100]$ ,  $y \parallel [010]$ , and  $z \parallel [001]$ , with carrier transport along the  $x$ -direction. A supercell is then generated by repeating the simulation cell along the transport direction. We divide the resulting supercell into source, channel, and drain regions. To incorporate alloy-scattering effects, we randomly rearrange Si and Ge atoms in the channel region while keeping their numbers fixed to preserve the target composition.

For each combination of channel length (3, 4, and 5 nm) and Ge mole fraction (12.5, 25, and 50%), we generate seven random-alloy samples with different atomic configurations, resulting in a total of 63 samples.

All generated supercells are structurally relaxed using the SIESTA package [7] within the generalized gradient approximation and the Perdew–Burke–Ernzerhof exchange–correlation functional until the maximum residual force is below 0.05 eV/Å. The DFT Hamiltonians extracted from the relaxed structures are subsequently projected onto a reduced mode-space basis. Using the supercell mode-space method [8], each Hamiltonian is compressed to less than 5% of its original size, thereby significantly reducing the computational cost of the NEGF calculations. Within 0.15 eV below the valence-band maximum ( $E_V$ ), the transmission of the reduced Hamiltonian is calculated at  $(k_y, k_z)$  points using our in-house NEGF solver. The bulk transmission is

$$TR_{\text{bulk}}(E) = \frac{1}{(2\pi)^2} \iint TR(E, k_y, k_z) dk_y dk_z. \quad (1)$$

In practice, using the symmetry of  $TR(k_y, k_z) = TR(-k_y, -k_z)$ , we have used only 13 points of the 25  $k$ -points as shown in Fig. 2(a) and (b).

For each Ge mole fraction and channel length  $L$ , the resistance is calculated from the bulk transmission using the Landauer formula:

$$\begin{aligned} \frac{1}{R(L)} &= G(L) \\ &= \frac{2q^2}{h} \int \langle TR_{\text{bulk}}(E, L) \rangle \left( -\frac{\partial f(E, E_F, T)}{\partial E} \right) dE. \end{aligned} \quad (2)$$

where  $R$  is the resistance,  $G$  is the conductance,  $q$  is the elementary charge,  $h$  is Planck's constant,  $f(E, E_F, T)$  is the Fermi–Dirac distribution, and  $\langle TR_{\text{bulk}}(E, L) \rangle$  denotes the average bulk transmission obtained from multiple random-alloy configurations.

As shown in Fig. 3(a), the resistance calculated from the bulk transmission exhibits a linear increase with channel length for a given Ge fraction. Based on this linear relationship, the hole mobility is extracted using the  $dR/dL$  method:

$$\mu_{\text{alloy}} = \frac{1}{qp\rho} = \left( \frac{dR}{dL} \right)^{-1} \frac{1}{qpA}, \quad (3)$$

where  $\mu_{\text{alloy}}$  is the alloy-scattering-limited mobility,  $p$  is the hole density,  $\rho$  is the resistivity, and  $A$  is the cross-sectional area. As shown in Fig. 3(b), the calculated mobility remains nearly constant at low hole density and decreases noticeably above  $\sim 10^{19} \text{ cm}^{-3}$  due to enhanced alloy scattering in deeper valence-band states, consistent with the general mobility trend. Moreover, the total mobility obtained by combining the calculated alloy-scattering-limited mobility with the phonon-limited mobility [9] through Matthiessen's rule reproduces the overall dependence of the Hall mobility on Ge mole fraction reported in Ref. [10] (Fig. 4).

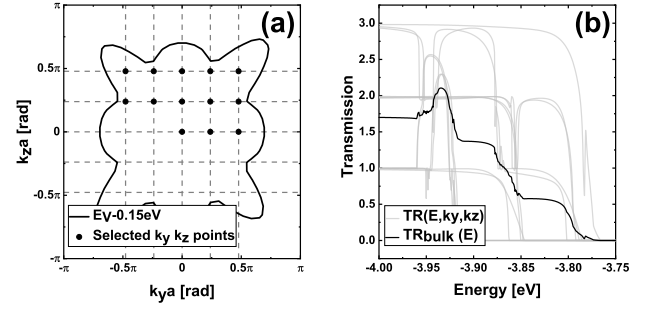


Fig. 2. (a) Constant-energy contour corresponding to 0.15 eV below the  $E_V$  in the Brillouin zone (black line) with selected  $(k_y, k_z)$  points (black dots). (b) Transmission as a function of energy for individual  $(k_y, k_z)$  points (gray lines) and the corresponding averaged bulk transmission (black line) for a single random sample.

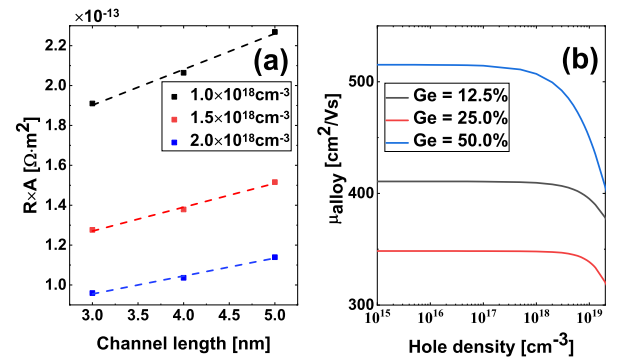


Fig. 3. (a) Resistance–area product ( $R \cdot A$ ) as a function of channel length for hole densities of  $1.0 \times 10^{18}$ ,  $1.5 \times 10^{18}$ , and  $2.0 \times 10^{18} \text{ cm}^{-3}$  for Ge mole fraction of 25%. The dashed lines represent linear fits to the calculated data points. (b) Alloy-scattering-limited hole mobility as a function of hole density with Ge mole fractions of 12.5, 25.0, and 50.0%.

### III. ABSOLUTE POTENTIAL MODEL

While DFT is rigorous, its high computational cost makes it unsuitable for extensive random sampling and large-scale device simulation. To overcome this limitation, we develop the  $3 \times 3$   $k \cdot p$ -based model Hamiltonian that replaces the full DFT Hamiltonian in NEGF transport calculations. The model Hamiltonian consists of the virtual crystal approximation Hamiltonian ( $H_{\text{VCA}}$ ) and the atom-type-dependent absolute potential ( $V_{\text{APM}}$ ) as

$$H = H_{\text{VCA}} + V_{\text{APM}}. \quad (4)$$

In this work, the  $H_{\text{VCA}}$  is described by the  $3 \times 3$  Dresselhaus–Kip–Kittel (DKK)  $k \cdot p$  Hamiltonian [11],

$$\begin{aligned} H_{\text{VCA}}(\mathbf{k}) &= \begin{pmatrix} \Theta_x & Nk_x k_y & Nk_x k_z \\ Nk_y k_x & \Theta_y & Nk_y k_z \\ Nk_z k_x & Nk_z k_y & \Theta_z \end{pmatrix}, \quad (5) \\ \Theta_x &= Lk_x^2 + M(k_y^2 + k_z^2), \\ \Theta_y &= Lk_y^2 + M(k_x^2 + k_z^2), \\ \Theta_z &= Lk_z^2 + M(k_x^2 + k_y^2). \end{aligned}$$

The parameters  $L$ ,  $M$ ,  $N$  and lattice constant are extracted from the DFT calculations.

Although  $H_{VCA}$  reproduces the composition-averaged valence-band dispersion of SiGe, it does not contain the local potential fluctuation arising from the random distribution of Si and Ge atoms. As a result, the periodically repeated  $H_{VCA}$  alone cannot describe the alloy-scattering-induced reduction of transmission in NEGF calculation. To capture this effect, Si and Ge potentials are assigned on a three-dimensional finite-difference grid. These potentials mimic the local potential fluctuations caused by the actual atomic configuration (Fig. 5(d) and (e)). The model potential evaluated at the  $i$ -th real-space grid point is written as

$$V_{APM}(\mathbf{r}_i) = \left( \sum_{\alpha=1}^{N_{\text{atom}}} v(r_{i\alpha}) \right) \mathbf{I}_{3 \times 3}, \quad r_{i\alpha} = |\mathbf{r}_i - \mathbf{R}_\alpha|. \quad (6)$$

where  $\mathbf{I}_{3 \times 3}$  is the  $3 \times 3$  identity matrix,  $\alpha$  is an index of the virtual Si or Ge atoms,  $\mathbf{R}_\alpha$  is the position of the  $\alpha$ -th atom,  $\mathbf{r}_i$  is the position of the  $i$ -th real-space grid point. The potential contribution from atom type  $s \in \{\text{Si}, \text{Ge}\}$  is defined as

$$v(r) = v_s(r) = \begin{cases} A_s \exp\left(-\frac{r^2}{2\sigma_s^2}\right), & r \leq r_{c,s}, \\ 0, & r > r_{c,s}. \end{cases} \quad (7)$$

where  $A_s$  determines the peak amplitude of the potential,  $\sigma_s$  controls its spatial width, and  $r_{c,s}$  is the cutoff radius. The model potential evaluated on the real-space grid is added to the on-site diagonal elements of the Hamiltonian. The random arrangement of virtual Si and Ge atoms in the channel region incorporates alloy disorder effect into the Hamiltonian, enabling our model to describe the physical picture where alloy scattering originates from potential disorder caused by the potential difference between Si and Ge atoms. All subsequent transport calculations are performed using the same procedure as in the DFT-based workflow as shown in Fig. 1.

We calibrate the parameters of  $V_{APM}$  to match the DFT transmission results for each Ge composition. As shown in Fig. 5(a)–(c), the calibrated model shows good agreement with the DFT transmission results. The lower computational cost of the model compared with DFT is a critical enabling technology for device-level simulations, which requires a large number of statistical samples to accurately describe alloy scattering in realistically sized transistors.

## CONCLUSION

In this study, we establish a first-principles-based framework for evaluating alloy-scattering-limited hole mobility in bulk SiGe. The calculated mobility shows good agreement with trends reported in both experiments and previous simulations, demonstrating the predictive capability of the proposed approach. To extend the accuracy of DFT-based NEGF calculations to computationally demanding statistical sampling and large-scale device simulations, we develop a  $k \cdot p$ -based

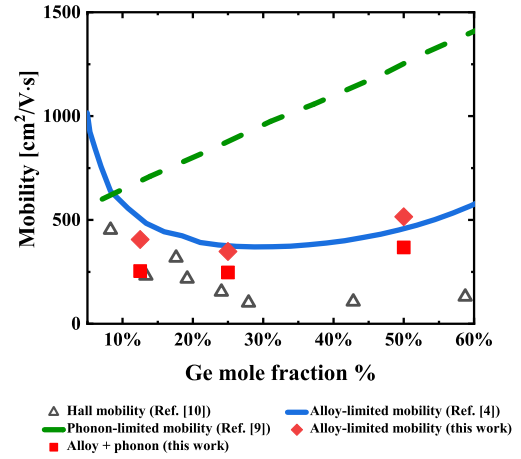


Fig. 4. Mobility as a function of Ge mole fraction. The total mobility is evaluated using Matthiessen's rule by combining the alloy-limited mobility calculated in this work with the phonon-limited mobility taken from Ref. [9].

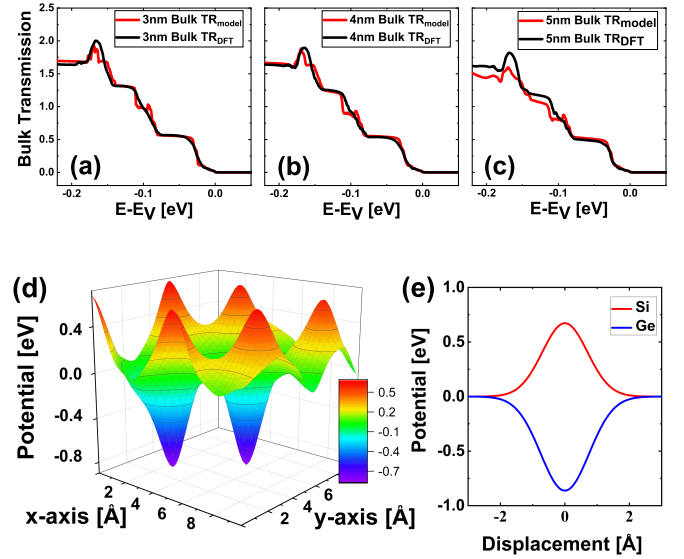


Fig. 5. Comparison of the bulk transmission averaged over random atomic configurations for a Ge mole fraction of 25% and channel lengths of (a) 3 nm, (b) 4 nm, and (c) 5 nm. (d) Potential profile on a  $z$  cross sectional plane of the unit cell used in the absolute potential model. (e) Atomic potential profiles of Si and Ge used in the absolute potential model.

absolute potential model that faithfully reproduces the first-principles-based transmission characteristics at a substantially reduced computational cost. This enables practical mobility evaluation over many random-alloy configurations and provides a scalable pathway toward large-scale device level transport simulations while retaining first-principles-level accuracy.

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