

Bridging Semiconductor Physics and Device Engineering: From Crystal Anisotropy to Efficient Quantum Transport

Nobuya Mori

Graduate School of Engineering, The University of Osaka

Suita, Osaka, Japan

nobuya.mori@eei.eng.osaka-u.ac.jp

Abstract—This paper revisits the physical foundations of quantum transport in anisotropic low-dimensional semiconductors from the viewpoints of carrier dynamics, mobility theory, and electron-phonon interaction. We first show that finite intersubband Berry connections arising from off-diagonal effective-mass fundamentally modify electron dynamics. A rigorous treatment based on the Krieger-Iafrate equation demonstrates that electrons initially accelerate according to the bulk dispersion rather than the conventional low-dimensional subband dispersion. We further show that the Berry connection introduces an additional velocity component, leading naturally to a unified description of carrier mobility that continuously bridges the bulk and strong-confinement limits.

We also investigate acoustic deformation-potential scattering by simultaneously incorporating deformation-potential anisotropy, anisotropic elasticity, and interface-modulated phonon modes. The results demonstrate that crystal anisotropy substantially alters the effective deformation potential and should therefore be incorporated into quantitative mobility modeling.

These results suggest that quantum-geometry physics and crystal anisotropy are not merely corrections to conventional effective-mass theory but constitute fundamental ingredients of a unified framework for next-generation quantum transport simulations spanning semiclassical and atomistic approaches.

Index Terms—acoustic phonon scattering, Berry connection, carrier mobility, crystal anisotropy, effective-mass theory, nanosheet transistor, quantum transport

I. INTRODUCTION

The continuous scaling of semiconductor devices has fundamentally changed the role of crystal anisotropy in carrier transport. Whereas electron transport properties in bulk silicon are nearly isotropic owing to the cubic crystal symmetry and the equivalent contributions of the six conduction-band valleys, reduced dimensionality in metal-oxide-semiconductor (MOS) inversion layers, nanowires, and nanosheet transistors breaks this symmetry and allows the intrinsic anisotropy of the electronic structure to directly govern macroscopic transport properties. Consequently, understanding how crystal anisotropy influences carrier dynamics has become one of the central issues in modern semiconductor device physics.

Two distinct forms of anisotropy become important in low-dimensional semiconductor structures. The first originates from the electronic structure itself and is manifested through the anisotropic effective-mass tensor and the associated Berry connection. The second originates from the crystal elasticity

governing acoustic phonons and their interaction with electrons. Although these two aspects have traditionally been investigated independently, they both arise from the same underlying crystal symmetry and together determine carrier transport in devices.

The physical origins of these phenomena were established in a series of pioneering studies carried out between the 1950s and the 1970s. Herring and Vogt incorporated deformation-potential and sound-velocity anisotropy into mobility calculations for bulk silicon [1]. Stern and Howard established the effective-mass theory for two-dimensional electron gases with arbitrary crystallographic orientations [2], whereas Ezawa clarified the role of interface-modulated acoustic phonons in silicon inversion layers [3]. These classical theories continue to provide the basis of modern device simulation.

In this paper, we revisit the physical foundations of quantum transport in anisotropic low-dimensional semiconductors by incorporating modern physical and engineering perspectives. We first demonstrate how the Berry connection arising from off-diagonal effective-mass components fundamentally modifies carrier dynamics and mobility. We then discuss the influence of crystal anisotropy on acoustic deformation-potential scattering and its implications for mobility modeling. Finally, we briefly outline recent efforts toward efficient atomistic quantum transport simulations based on the R-matrix theory [4], [5] and the equivalent model [6], [7]. Together, these studies point toward a unified physical framework that bridges semiclassical and atomistic descriptions of quantum transport in anisotropic low-dimensional systems.

II. CARRIER DYNAMICS WITH OFF-DIAGONAL EFFECTIVE MASSES

The effective-mass approximation has long served as the standard framework for describing carrier transport in semiconductor nanostructures. Within this framework, carrier dynamics are usually assumed to be completely determined by the subband dispersion relation. This assumption is valid when the reciprocal effective-mass tensor is diagonal. However, once off-diagonal effective-mass (ODEM) components become finite, the electronic eigenstates acquire a non-trivial $\mathbf{k}$ -dependence that gives rise to a finite intersubband Berry connection (ISBC). As shown below, this Berry connection

fundamentally modifies both the free-flight dynamics and the mobility of low-dimensional electron systems.

We first consider a two-dimensional electron gas (2DEG) confined in the z direction by a confinement potential $V(z)$. For a conduction-band valley characterized by the reciprocal effective-mass tensor w_{ij} , the envelope function satisfies

$$\left[\frac{1}{2} \sum_{ij} w_{ij} p_i p_j + V(z) \right] \psi(x, y, z) = E \psi(x, y, z), \quad (1)$$

where $p_x = -i\hbar(\partial/\partial x)$, and similarly for p_y and p_z . The eigenfunctions and eigenvalues for (1) were derived by Stern and Howard [2]:

$$\psi_{n\mathbf{k}}(x, y, z) = \zeta_n(z) e^{-iz(w_{xz}k_x + w_{yz}k_y)/w_{zz}} e^{i\mathbf{k} \cdot \mathbf{x}}, \quad (2)$$

$$E_{n\mathbf{k}} = E_n + \frac{1}{2} \hbar^2 \left[\left(w_{xx} - \frac{w_{xz}^2}{w_{zz}} \right) k_x^2 + \left(w_{yy} - \frac{w_{yz}^2}{w_{zz}} \right) k_y^2 + 2 \left(w_{xy} - \frac{w_{xz}w_{yz}}{w_{zz}} \right) k_x k_y \right]. \quad (3)$$

where n is the subband index, $\mathbf{k} = (k_x, k_y)$ is the in-plane wave vector, $\mathbf{x} = (x, y)$ is the in-plane position vector, $\zeta_n(z)$ is the subband wavefunction, and E_n is the subband energy level. The off-diagonal elements of the reciprocal effective-mass tensor appear only through a phase factor of the wavefunction, whereas the energy dispersion is modified by a quadratic correction. By introducing the vector $\gamma = (w_{xz}/w_{zz}, w_{yz}/w_{zz})$, these eigenfunctions and eigenvalues can be concisely expressed as

$$\psi_{n\mathbf{k}}(x, y, z) = u_{n\mathbf{k}}(z) e^{i\mathbf{k} \cdot \mathbf{x}}, \quad (4)$$

$$E_{n\mathbf{k}} = E_n + E_{2D}(\mathbf{k}), \quad (5)$$

where $u_{n\mathbf{k}}(z)$ and $E_{2D}(\mathbf{k})$ are defined as

$$u_{n\mathbf{k}}(z) = e^{-iz\gamma \cdot \mathbf{k}} \zeta_n(z), \quad (6)$$

$$E_{2D}(\mathbf{k}) = E_{3D}(\mathbf{k}) - \frac{1}{2} \hbar^2 w_{zz} (\gamma \cdot \mathbf{k})^2, \quad (7)$$

and

$$E_{3D}(\mathbf{k}) = \frac{1}{2} \hbar^2 (w_{xx}k_x^2 + 2w_{xy}k_xk_y + w_{yy}k_y^2). \quad (8)$$

The phase factor in (6) has a profound physical consequence. Because $u_{n\mathbf{k}}(z)$ explicitly depends on the in-plane wave vector, a finite ISBC naturally emerges,

$$\mathbf{A}_{mn} = \langle u_{m\mathbf{k}} | i \nabla_{\mathbf{k}} | u_{n\mathbf{k}} \rangle = \langle \zeta_m | z | \zeta_n \rangle \gamma. \quad (9)$$

Unlike the Berry curvature, which vanishes owing to time-reversal symmetry in the present system, the ISBC remains finite whenever both $\gamma \neq 0$ and $\langle \zeta_m | z | \zeta_n \rangle \neq 0$. It therefore provides the microscopic origin of intersubband coupling during carrier acceleration. This observation immediately indicates that the conventional picture of carrier motion solely along the subband dispersion is incomplete. Instead, the electron wave packet continuously exchanges amplitudes among different subbands during acceleration, even in the absence of scattering, as shown below.

Equation (7) suggests that the in-plane effective mass obtained from the confined subband dispersion is always larger

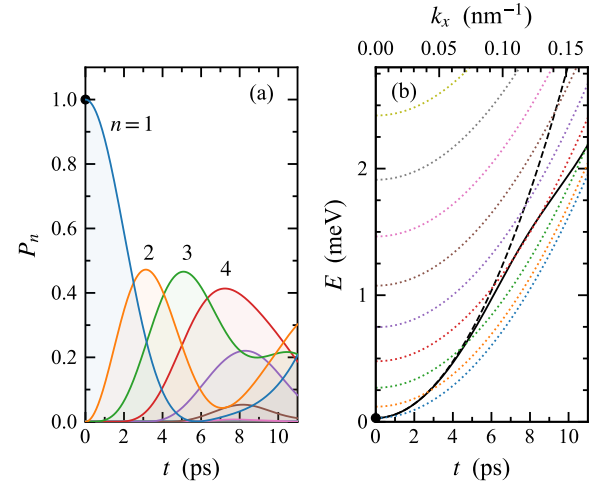


Fig. 1. (a) Time evolution of the probability $P_n(t)$ of finding an electron in the n th subband for a 200 nm-thick silicon plate with a (110) surface under an electric field of $F_x = 0.1$ kV/cm applied along the $[1\bar{1}0]$ direction. The filled symbol ($\bullet$) indicates the initial condition, $P_n(0) = \delta_{n,1}$. (b) Corresponding effective dispersion $\bar{E}(\mathbf{k}(t))$ [10] (solid curve) for an electron initially at $\mathbf{k} = 0$, together with the bulk dispersion (dashed curve) and the 2DEG subband dispersions (dotted curves).

than that of the bulk crystal whenever $\gamma \neq 0$. If the subband dispersion alone governed carrier dynamics, electrons would always accelerate according to $E_{2D}(\mathbf{k})$. Surprisingly, this is not the case. As demonstrated by Esseni and Palestri [8], when $\mathbf{A}_{mn} \neq 0$, transitions between the m th and n th subbands occur during free flight, meaning electrons do not necessarily accelerate strictly along $E_{2D}(\mathbf{k})$. The breakdown of this intuitive picture can be demonstrated rigorously using the Krieger-Iafrate equation [9], which provides the exact time evolution of electrons under a uniform electric field. The calculation reveals that electrons initially accelerate according to the bulk dispersion rather than the confined subband dispersion [10]. Figure 1 provides direct evidence of this behavior. The occupation probabilities evolve coherently owing to the finite Berry connection, and the corresponding effective dispersion follows the bulk dispersion during the initial stage of acceleration before gradually approaching the confined 2DEG dispersion. The physical implication is significant. The conventional free-flight model employed in semiclassical Monte Carlo simulations assumes that electrons always propagate along the subband dispersion. For systems possessing finite ODEM components, this assumption should be replaced by a description that explicitly accounts for coherent intersubband dynamics through the Berry connection.

III. BERRY-CONNECTION CONTRIBUTION TO CARRIER MOBILITY

The previous section demonstrated that finite ISBCs modify the free-flight dynamics of electrons. An equally important consequence is that they also contribute directly to carrier mobility. Conventional mobility theories implicitly assume that the carrier velocity is completely determined by the energy

dispersion. However, this assumption is no longer valid in the presence of ODEM components. The Berry connection introduces an additional velocity arising from coherent inter-subband coupling, thereby modifying the transport coefficients even within the linear-response regime.

The conventional expression for low-field mobility is obtained by evaluating the linear response of the carrier velocity to an applied electric field. Within the effective-mass approximation, the velocity operator is usually identified with the gradient of the subband dispersion, leading naturally to the familiar conductivity formula. This picture implicitly assumes that carriers remain in a subband during acceleration. When finite ISBCs exist, this assumption breaks down because the electronic wavefunction continuously evolves among different subbands. Consequently, the carrier velocity contains an additional contribution, proportional to A_{mn} , that is absent from conventional transport theories.

Assuming a relaxation time τ and evaluating the mobility μ of a 2DEG using the Kubo formula, μ can be expressed as the sum of two terms: μ_{intra} (determined by the band gradient) and μ_{inter} (determined by A_{mn}). Here, $\mu_{\text{intra}} = e\tau/m_{2D}$ with m_{2D} being the effective mass given by the curvature of $E_{2D}(\mathbf{k})$. In the limit of strong confinement or weak scattering, the contribution of μ_{inter} becomes negligible, yielding $\mu = \mu_{\text{intra}} + \mu_{\text{inter}} \approx e\tau/m_{2D}$, which corresponds to the mobility determined by the 2DEG dispersion relation. Conversely, in the limit of weak confinement or strong scattering, $\mu = \mu_{\text{intra}} + \mu_{\text{inter}}$ approaches $e\tau/m_{3D}$, which is determined by the bulk in-plane dispersion. In this limit, the system mobility should naturally converge to the bulk mobility, highlighting the necessity of accounting for velocity components arising from the Berry connection when modeling mobility in systems with non-zero ODEM. This result resolves a long-standing inconsistency between the bulk and two-dimensional effective-mass descriptions. The present formulation demonstrates that they are continuously linked through the Berry connection.

These results indicate that carrier mobility in anisotropic low-dimensional semiconductors should be viewed as a manifestation of quantum geometry rather than solely as a consequence of the energy dispersion. The present theory therefore provides a unified physical description of carrier transport spanning the bulk, weak-confinement, and strong-confinement regimes within a single quantum-mechanical framework.

IV. CRYSTAL ANISOTROPY AND ACOUSTIC-PHONON SCATTERING

The previous sections focused on electronic anisotropy arising from the effective-mass tensor and the associated Berry connection. Carrier transport, however, is governed not only by free-flight dynamics but also by scattering processes. Among various scattering mechanisms, acoustic phonon scattering constitutes one of the most fundamental mobility-limiting mechanisms at room temperature. Consequently, a complete transport theory must consistently account for crystal anisotropy in both electron dynamics and electron-phonon interaction.

In conventional device modeling, an isotropic effective deformation potential D_{ac} and an isotropic longitudinal sound velocity v_ℓ are usually assumed, and the scattering probability is modeled to be proportional to $(D_{\text{ac}}/v_\ell)^2$. However, the Δ valleys of the silicon conduction band exhibit anisotropy, and the second-rank deformation potential tensor Ξ_{ij} possesses anisotropy characterized by the dilatation component Ξ_d and the shear component Ξ_u [1]. Furthermore, calculating the Zener anisotropy factor from the elastic stiffness constants c_{11} , c_{12} , and c_{44} [11], which characterize the elastic properties of cubic semiconductors, yields $A = 2c_{44}/(c_{11} - c_{12}) = 1.56$, indicating that silicon cannot be treated as an isotropic elastic body. Unlike in isotropic elastic media, acoustic phonon modes are divided into quasi-longitudinal, quasi-transverse, and pure transverse modes, and electrons interact with two types of phonon modes: quasi-longitudinal and quasi-transverse. Moreover, their sound velocities vary depending on the crystallographic orientation. Furthermore, when an interface is present, such as in MOS structures, these acoustic modes hybridize, resulting in a complex dispersion relation [12].

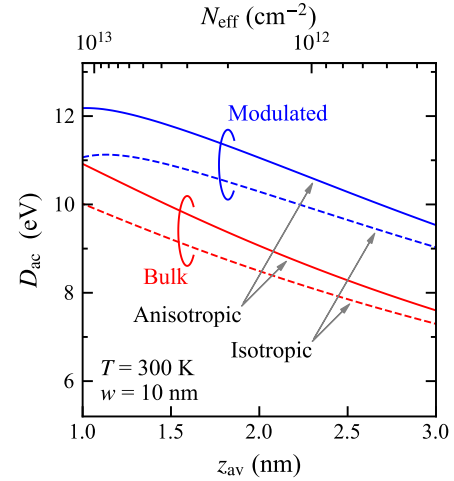


Fig. 2. Effective deformation potential D_{ac} as a function of the average distance of the electron from the interface, z_{av} ($= 3/b$). The blue solid (dashed) curve represents D_{ac} for the modulated phonon model with anisotropic (isotropic) elasticity, while the red solid (dashed) curve represents D_{ac} for the bulk phonon model with anisotropic (isotropic) elasticity. The upper horizontal axis indicates the effective sheet electron density, $N_{\text{eff}} = b^3 \hbar^2 \epsilon / 12 m_\ell e^2$.

Figure 2 summarizes the calculated effective acoustic deformation potential D_{ac} in a silicon-on-insulator (SOI) using the method of [12]. The value of D_{ac} was determined such that the mobility calculated by considering the deformation potential anisotropy, crystal anisotropy, and phonon modulation effects equals that calculated assuming an isotropic deformation potential D_{ac} and an isotropic sound velocity v_ℓ . Here, the isotropic sound velocity v_ℓ was taken as the average sound velocity $v_\ell = (c_\ell/\rho)^{1/2}$, where ρ is the density of the silicon crystal, $c_\ell = c_{12} + 4c_{44} + (3/5)c^*$, and $c^* = c_{11} - c_{12} - 2c_{44}$. The modulated phonon modes were obtained by solving the Christoffel equation [13] assuming a (001) silicon plate of thickness w . Regarding the electronic states, only the lowest

subband was considered, and a Fang-Howard-type wavefunction $\zeta(z) \propto z \exp(-bz/2)$ was assumed. Unlike the symmetric quantum well model discussed in [12], electrons in the present model interact with both symmetric and antisymmetric phonon modes. The deformation potential constants Ξ_d and Ξ_u were taken from the values reported by Fischetti and Laux [14]. The results calculated assuming bulk phonons and/or an isotropic crystal are also plotted in the figure. The isotropic crystal model assumes elastic stiffness constants of $\hat{c}_{11} = c_\ell$, $\hat{c}_{12} = c_\ell - 2c_t$, and $\hat{c}_{44} = c_t$, with $c_t = c_{44} + (1/5)c^*$. We see that both the phonon modulation and the crystal anisotropy have non-negligible effects on D_{ac} . The calculated deformation potential exhibits a pronounced dependence on the average electron position, demonstrating that the scattering strength cannot be regarded as a material constant in confined structures. Note that only the lowest subband is considered in Fig. 2, with higher subbands neglected. The latter should be taken into account under larger z_{av} or weak confinement.

V. TOWARD LARGE-SCALE QUANTUM TRANSPORT SIMULATION

The preceding sections have revisited the physical foundations of carrier transport in anisotropic low-dimensional semiconductors within the framework of the effective-mass approximation, playing a vital role in mobility modeling and semiclassical transport simulations. While the effective-mass approximation provides deep physical insights into carrier dynamics and scattering, it inherently struggles to fully capture crystal anisotropy and complex band-mixing effects in ultra-scaled geometries, necessitating atomistic approaches. Such atomistic-based modeling and simulation are expected to become increasingly important when analyzing ultra-scaled devices featuring complex geometries or novel materials. However, given current computational power and numerical algorithms, analyzing realistic device structures within reasonable computation times remains challenging. Consequently, improving the efficiency and speed of atomistic simulation methods is also an urgent priority.

Among various numerical approaches, the R-matrix method [4], [5] provides an attractive framework because it naturally separates the calculation of the closed-system eigenstates from the open-boundary scattering problem. This formulation enables efficient evaluation of quantum transport while preserving the physical transparency of wavefunction-based descriptions.

The computational efficiency can be further improved by introducing the equivalent model [6], [7], a low-rank representation of the transport Hamiltonian. Instead of solving the full atomistic problem, the essential transport physics is projected onto a reduced basis while maintaining high accuracy within the energy window of interest. Unlike conventional mode-space approaches, the present approach does not assume the lower bound of the energy spectra. The reduced basis is constructed so as to preserve the quantum states that dominate transport, thereby providing both computational efficiency and physical interpretability.

VI. CONCLUSION

This paper has revisited the physical foundations of carrier transport in anisotropic low-dimensional semiconductors from the viewpoints of carrier dynamics, mobility theory, electron-phonon interaction, and large-scale quantum transport simulation.

We have shown that finite off-diagonal effective-mass components generate intersubband Berry connections that fundamentally modify electron dynamics. The resulting quantum geometry introduces an additional contribution to the carrier velocity, providing a unified description of transport from the bulk limit to strongly confined systems.

We have also demonstrated that crystal anisotropy plays an equally important role through acoustic deformation-potential scattering. The effective deformation potential is strongly influenced by elastic anisotropy and interface-modulated phonon modes and should therefore be regarded as an effective transport parameter rather than an intrinsic material constant.

Finally, we discussed recent developments in efficient quantum transport simulation based on the R-matrix method and the equivalent model, highlighting the importance of combining physically sound transport theory with scalable numerical algorithms.

Taken together, these results suggest that carrier transport in low-dimensional semiconductors should be understood as a consequence of quantum geometry and crystal anisotropy acting simultaneously. Rather than representing incremental corrections to conventional effective-mass theory, these concepts constitute essential ingredients of a unified physical framework for next-generation semiconductor transport modeling.

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