I. INTRODUCTION

Non-planar transistor channels used in tri-gate [1] or gate-all-around (GAA) [2] device architectures offer superior electrostatic control, which reduces short-channel effects. The limiting factor in these devices is surface-roughness scattering (SRS) as it is more pronounced in these devices than in planar technologies, which has two reasons: one is that there are more surfaces to scatter off and the other is that sidewall roughness or line-edge-roughness (LER) are harder to control in the fabrication process.

Being of such importance it is surprising to find that a thorough perturbative treatment of SRS is missing in literature. Most low-field mobility calculations for non-planar channels employ phenomenological descriptions or extensions of SRS models for planar structures. Commonly, tri-gate channels are modeled as three separate non-interacting planar channels at the top and each sidewall, and the scattering rate in GAA channels is assumed to be proportional to $d^6$, with $d$ being the diameter. The latter is based on an analysis of quantum wells in Ref. [3].

The only work known to us that rigorously treats SRS for a one-dimensional electron gas (1DEG) is Ref. [4]. The authors calculate the electron mobilities of gated silicon nanowires taking into account both axial and angular interaction of electrons with the rough nanowire surface. The calculations, however, rely on cylindrical symmetry of both real and k-space; this means that first, the model cannot be extended to non-cylindrical geometries, and second, that band anisotropy is completely neglected. The authors approximate the effective masses of (100)-oriented nanowires as isotropic in the cross-section, which is questionable in itself and fails to capture the effect of channel orientation. Channel orientation is likely to play an important role in SRS as experimental data from [5] indicates.

This raises the following issues and questions:

- Rotational symmetry even of cylindrical GAA channels is not likely to be valid and must be dropped.
- The $d^6$-approximation is only valid in very narrow channels with very low electric fields in the cross-section.
- How to define a “diameter” for a tri-gate device, especially in the presence of electrostatic confinement?
- How can SRS theory for planar and cylindrical geometries be extended to more general surfaces, that don’t even need to be closed shapes?

In this work, we investigate the effect of band structure anisotropy and channel orientation on SRS in non-planar channels such as tri-gate and GAA structures. A new formalism is introduced for calculating SRS rates for non-planar structures.

II. THEORY

We start by writing the ensemble average of the surface-roughness-induced transition rate for a one-dimensional carrier gas as

$$\langle S_{n,n'}(k,k') \rangle = \frac{2\pi}{\hbar} |\langle H_{n,n',k,k'} \rangle|^2 \delta(E(k) - E(k')), \quad (1)$$

from state $n$ to $n'$ and from one-dimensional k-vector $k$ to $k'$. To evaluate the matrix element $H_{n,n',k,k'}$ we take a look at the perturbing potential in Fig. 1. The position of an abrupt potential step of height $\Delta V$ fluctuates as described by the function $\Delta(r)$. The resulting perturbation potential is a narrow barrier or well – depending in the sign of $\Delta(r)$. To evaluate the matrix element $H_{n,n',k,k'}$, we approximate the perturbing potential by a weighted surface-delta-distribution $\Delta(r)\delta(r \in \mathcal{S})$, where $\mathcal{S}$ represents the points of the ideal surface. This allows us to convert the evaluation the matrix element $H_{n,n',k,k'}$ from a volume integration to a surface integration,

$$H_{n,n',k,k'} = \Delta V \int_{\mathcal{S}} \psi^*_{n,k}(r) \psi_{n',k'}(r) \Delta(r) \, dA. \quad (2)$$

The matrix element (2) cannot be evaluated directly since $\Delta(r)$ is a random function. Instead, $\Delta(r)$ is characterized by its autocorrelation function $c(r) = \langle \Delta(r)\Delta(r+r) \rangle$ and its 2D Fourier transform $C(q)$, i.e. the roughness “power spectrum”. We make no assumptions about the nature of $c(r)$ or $C(q)$ in this work, but an exponential autocorrelation function $c(r) = \Delta^2 \exp(-r/\Lambda)$ is considered to represent the properties of a rough surface/interface [8] correctly. In the frame of reference of a propagating electron, surface roughness appears as an ensemble of surface-bound phonons with zero frequency and a momentum distribution according to $C(q)$. 

The formalism is an extension of the theory by Prange and Nee [6] for planar structures, which has been widely used for calculating the conductivity of inversion layers and thin films [7]. We derive matrix elements for open and closed surfaces of arbitrary shape taking anisotropy of the band structure fully into account. Numerical experiments performed on tri-gate and GAA cross-sections indicate that SRS is greatly influenced by band anisotropy and channel orientation.
The ensemble average of the square magnitude of (2) can be evaluated.

\[ \left\langle |H_{n,n',k,k'}|^2 \right\rangle = \frac{1}{2\pi L^2} \int_{C} \int_{s} f_{n,n',k,k'}(s) \overline{f_{n,n',k,k'}(s')} \Delta \langle \Delta(r) \Delta(r') \rangle \] (3)

So far we have made no assumptions about the electron states \( \psi_{n,k} \). The carriers form a one-dimensional gas and are confined in two spatial dimensions as shown in Fig. 2. We separate the electron states into a two-dimensional standing wave along the channel axis.

Using this separation approach, we can rewrite (3) as

\[ \left\langle |H_{n,n',k,k'}|^2 \right\rangle = \frac{1}{2\pi L^2} \int_{C} \int_{s} f_{n,n',k,k'}(s) \overline{f_{n,n',k,k'}(s')} e^{i(k-k')(z-z')} \Delta \langle \Delta(r) \Delta(r') \rangle dz' dz ds ds'. \] (4)

The integration across surface \( \mathcal{C} \) was separated into integrations along curve \( \mathcal{C} \), i.e. the intersection of \( \mathcal{C} \) with the cross-section plane, and a length \( L \) along the channel direction; \( s \) denotes the path coordinate along the curve and \( z \) the axial coordinate. We introduced the form functions \( f_{n,n',k,k'}(s) \) which are defined as

\[ f_{n,n',k,k'}(s) = \psi^*_{n,k} \psi_{n',k'} \Delta V. \] (5)

The effect of different effective mass in the channel and the surrounding medium (gate dielectric) can be included in the form functions as

\[ f_{n,n',k,k'}(s) = \psi^*_{n,k} \psi_{n',k'}(V_n - V_{k'}) - \nabla \psi^*_{n,k} \cdot \nabla \psi_{n',k'} - \nabla \psi^*_{n,k} \cdot \nabla \psi_{n',k'} + \nabla \psi^*_{n,k} \cdot \nabla \psi_{n',k'}, \] (6)

where the subscripts \( + \) and \( - \) indicate either sides of the interface. In case the cross-section wavefunctions \( \psi_{n,k} \) do not penetrate into the surrounding medium, the expression in (6) can be approximated by

\[ f_{n,n',k,k'}(r) \approx \frac{\hbar^2}{2m_{\text{barrier}}} \left( \mathbf{n} \cdot \mathbf{m}_{\text{well}}^{-1} \cdot \nabla \psi^*_{n,k} \right) \left( \mathbf{n} \cdot \mathbf{m}_{\text{well}}^{-1} \cdot \nabla \psi_{n',k'} \right) \] (7)

Looking back at (4), we recall that \( \langle \Delta(r) \Delta(r') \rangle = c(r) \) and represent the autocorrelation as inverse 2D Fourier transform of the roughness power spectrum,

\[ c(r) = \frac{1}{4\pi^2} \int_{C} C(q)e^{iq_s(s-s')}e^{iq_z(z-z')} dq_s dq_z, \] (8)

separating the roughness “wave vector” \( q \) into an axial component \( q_s \) and a component \( q_z \) along \( \mathcal{C} \). Inserting (8) into (4), we arrive at

\[ \left\langle |H_{n,n',k,k'}|^2 \right\rangle = \frac{1}{4\pi^2 L^2} \int_{C} \int_{s} f_{n,n',k,k'}(s) \overline{f_{n,n',k,k'}(s')} C(q)e^{iq_s(s-s')}e^{iq_z(z-z')} \] (9)

Axial integration of the plane wave term \( e^{i(k-k'+q_1)(z-z')} \) leads to a \( 2\pi L \delta(k-k'+q_1) \) expression thus simplifying the previous equation to

\[ \left\langle |H_{n,n',k,k'}|^2 \right\rangle = \frac{1}{2\pi L} \int_{C} \int_{s} f_{n,n',k,k'}(s) \overline{f_{n,n',k,k'}(s')} C(q) \] (10)

A change of variables \( s' - s = s' \) gives

\[ \left\langle |H_{n,n',k,k'}|^2 \right\rangle = \frac{1}{2\pi L} \int_{C(q)} C(q) dq \] (11)

The term in square brackets represents an autocorrelation of the form functions \( f_{n,n',k,k'}(s) \) and the integration around it is a Fourier transform \( s \rightarrow q_s \). Using the Wiener-Khinchin theorem we can express the Fourier transform of the autocorrelation of \( f_{n,n',k,k'}(s) \) as square magnitude of its Fourier transform \( \mathcal{F}_{n,n',k,k'}(q_s) \) obtaining the final expression for the matrix element and transition rate,

\[ \left\langle |H_{n,n',k,k'}|^2 \right\rangle = \frac{1}{2\pi L} \int_{C(q)} C(q) dq \] (12)

\[ S_{n,n',k,k'} = \frac{1}{\hbar L} \int_{C(q)} C(q) dq \] (13)

A few assumptions are contained within this last step of our derivation:

- For closed curves \( \mathcal{C} \) (GAA channel) the Fourier transform is in fact a Fourier series expansion.
- For open curves \( \mathcal{C} \) (tri-gate channel) the wavefunctions are assumed to be square-integrable and so are the form functions \( f_{n,n',k,k'}(s) \). If the electrons are confined to the fin cross-section electrostatically, the value of \( f_{n,n',k,k'}(s) \) will exponentially decay for \( s \rightarrow \pm \infty \). This allows to extend the integration over \( \mathcal{C} \) to \( \mathbb{R} \).
- The roughness power spectrum is isotropic, \( C(q) = \hat{C}(q) \).

### III. Computation

The wavefunctions \( \psi \) are obtained by solving the closed-boundary Schrödinger equation in 2D in the parabolic band approximation,

\[ \frac{\hbar^2}{2} (\nabla \cdot m^{-1} \cdot \nabla + V) \psi = E \psi, \] (14)

with anisotropic effective mass tensor \( m \). The equation is discretized on an unstructured triangular mesh using a method.
reported earlier in [9]. The discretization ensures the correct
treatment of anisotropic bands and naturally includes the effect
of channel orientation. A self-consistent Schrödinger-Poisson
simulation is conducted to obtain the electron concentration in
the channel cross-section as well as the wavefunctions for each
valley and subband. The computed wavefunctions and energies
are used to compute the scattering rates between the subbands
which are then used to compute channel conductivities and
mobilities using the Kubo-Greenwood formula [10]. Fig. 3
outlines the computational procedure. 
Since we are assuming parabolic bands an energy-dependent
scattering rate from subband \( n \) to subband \( n' \) can be obtained
from (13) and the 1DEG density of states \( g_{1D,n'}(E) \),
\[
\frac{1}{\tau_{n,n'}(E)} = 1 \frac{1}{2\hbar} \int_{\mathbb{R}} |F_{n,n'}(q_\perp)|^2 C(q)dq_\perp g_{1D,n'}(E) \tag{15}
\]
An efficient procedure was devised to compute the spectral
form functions \( F_{n,n'}(q_\perp) \) required for the integral in (15).
The procedure is depicted in Fig. 4. The wavefunctions are used
to compute the form functions along the interface curve \( \varphi' \), which
are resampled onto an equidistant \( q_\perp \)-grid and fast-Fourier-
transformed to obtain their spectral counterparts \( \tilde{F}_{n,n'}(q_\perp) \).
Having found the spectral form functions \( \tilde{F}_{n,n'}(q_\perp) \) the
scattering rate in (15) is obtained via \( q_\perp \)-integration, visualized
in Fig. 5. The integral represents momentum conservation in
the cross-section plane. In a planar geometry with a two-
dimensional electron gas momentum conservation is charac-
terized by a \( \delta(k - k' + q) \) term. In a non-planar structure
cross-section momentum conservation is not sharply defined and
the \( \delta(k - k' + q) \) term is replaced by the integral in (15).
In addition to the SRS rate, the electron-phonon scattering
rates were also computed. Common literature parameters for
phonon scattering in bulk silicon were used with the exception
of the acoustic deformation potential, which was set to 14.6 eV
due to the proximity of the Si/SiO\(_2\) interface. All rough
surfaces were assumed to have exponential autocorrelation with
\( \Delta_{rms} = 0.48 \text{ nm} \) and \( \Lambda = 1.3 \text{ nm} \) [4].
All models were implemented as part of the Vienna
Schrödinger-Poisson quantum simulation framework [12].

IV. RESULTS
Using our model we investigated the properties of two sets
of devices. The first set consists of cylindrical GAA channels
of different diameters (3 nm to 14 nm) and orientations (\([100]\),
\([110]\), \([111]\)). For comparison, the \([100]\)-oriented channels
were also simulated with isotropic cross-section mass \( m_{tot} = 2m_1m_t/(m_1 + m_t) \) [4]. All channels were covered by 1 nm of
SiO\(_2\) as well as a metal gate. Fig. 6 shows the self-consistent
carrier concentration for the \([100]\) and \([110]\) channels at 1 V
gate bias. Except for ultra-thin channels of 4 nm and below the
carrier distribution is clearly anisotropic and one may expect
strong deviation from the isotropic approximation also in the
channel mobilities. This is in fact the case as seen in Fig. 7.
The deviation is especially strong for thicknesses around 5 nm
when gate bias is applied. This is the transition region between
bulk and layer inversion where a 2D quantum picture of the
channel cross-section is necessary. 

The second set of devices was constructed to match the
cross-section of Intel’s 22 nm node tri-gate transistors
[1]. Different combinations of channel/substrate orientation
(\([100])/(010), [110])/(001), [110])/(110), [110])/(111)) were evaluated.
Fig. 8 shows the self-consistent electron concentration for the
\([110])/(001)\) orientation. The electrons interact with an
Si/SiO\(_2\) curved interface comprised of a distribution of surface
orientations, which is different for every channel/substrate ori-
etnation. This results in heavily orientation-dependent channel
conductivity (Fig. 9).
We developed a new generic method for evaluating the surface-roughness-induced scattering rate in non-planar semiconductor structures. The method accurately captures band anisotropy and the roughness-induced momentum transfer between the confined states. Strong dependence of SRS-limited electron mobility on crystal orientation was observed with (100) and [110]/[110] being the optimal orientations.

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Fig. 7. Thickness-dependent mobilities for cylindrical GAA channels; left: (100) orientation unbiased; middle: 1 V gate bias, ■ – anisotropic bands, ● – isotropic approximation; the isotropic approximation deviates strongly from the anisotropic results; right: comparison of (100), (110), and (111) channels; solid lines – unbiased, dashed lines – 1 V gate bias.

Fig. 8. Left: TEM image of a tri-gate channel cross-section fabricated by Intel [1], segments of the computational domain are shown in color [13]. Right: Computed self-consistent electron concentration for a [110]/(001) channel/substrate orientation. The computational grid is visible as well.

Fig. 9. Channel conductivity vs. gate voltage for the device shown in Fig. 8. Different channel/substrate orientations show different behavior due to orientation-dependence of SRS.

V. CONCLUSION