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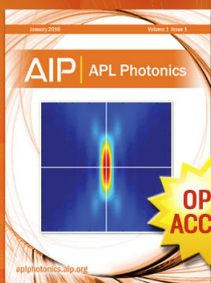
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Remote surface roughness scattering in fully depleted silicon-on-insulator devices with high- κ /SiO₂ gate stacks

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We investigate remote surface roughness (RSR) scattering by the SiO₂/HfO₂ interface in Fully Depleted Silicon-on-Insulator devices using Non-Equilibrium Green's Functions. We show that the RSR mobility is controlled by cross-correlations between the surface roughness profiles at the Si/SiO₂ and SiO₂/HfO₂ interfaces. Therefore, surface roughness and remote surface roughness cannot be modeled as two independent mechanisms. RSR tends to enhance the total mobility when the Si/SiO₂ interface and SiO₂ thickness profiles are correlated, and to decrease the total mobility when they are anti-correlated. We discuss the implications for the high- κ /Metal gate technologies.

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High- κ materials, such as HfO₂, have been introduced in Metal-Oxide-Semiconductor Field Effect Transistors in order to keep a tight electrostatic control over short channels while limiting gate leakage currents.¹ They usually remain separated from the channel by a thin interfacial layer (IL) of SiO₂. Yet the introduction of high- κ materials leads to a systematic decrease of carrier mobilities, which is very significant at weak inversion densities, but can persist in the strong inversion regime.²

Different scattering mechanisms have been put forward to explain this degradation. There is no doubt that charges trapped at the SiO₂/HfO₂ interface or in the HfO₂ layer (Remote Coulomb scattering (RCS)) make a major contribution at weak inversion.^{3–5} Remote scattering by polar optical phonons (RPH) in HfO₂ is also a serious candidate, especially in thin IL devices.^{5,6} Much less attention has been given up to now to scattering by roughness at the SiO₂/HfO₂ interface or equivalently by IL thickness fluctuations. At variance with RCS, this mechanism, known as remote surface roughness (RSR) scattering, is expected to be dominant in the strong inversion regime.

RSR has first been investigated with semi-classical Kubo-Greenwood approaches in a different context, namely, roughness at the SiO₂/Gate interface in polysilicon gate technologies.^{7–10} The models were later extended to HfO₂ and HfO₂/IL gate stacks.^{11,12} However, the different interfaces were assumed uncorrelated, and surface roughness (SR)/remote surface roughness modeled as two independent mechanisms.

In this letter, we use Non-Equilibrium Green's Functions (NEGF) methods^{13,14} to investigate RSR in the latest Fully Depleted Silicon-on-Insulator (FDSOI) thin-film technologies with high- κ /Metal gates. We show that RSR scattering is dominated by roughness at the SiO₂/HfO₂ interface, indeed prevails at large carrier densities (at variance with RCS), and decreases exponentially with IL thickness. More importantly, we demonstrate that the RSR correction is

controlled by cross-correlations between the Si/SiO₂ and SiO₂/HfO₂ interfaces. SR and RSR cannot, therefore, be modeled as two independent mechanisms. RSR is beneficial when the Si/SiO₂ interface and the IL thickness profiles are correlated, and detrimental if they are in anti-correlated.

Let us first discuss the basics of remote surface roughness scattering. The main effect of RSR is to modulate oxide thicknesses hence the effective field within the semiconductor. This gives rise to potential and charge fluctuations responsible for extra carrier scattering.^{7–12} In this picture, we expect stronger scattering from the SiO₂/HfO₂ interface than from the HfO₂/Metal gate interface, since the latter is usually much farther from the channel and is efficiently screened by the HfO₂ layer. This will indeed be confirmed by our numerical simulations on FDSOI devices. From now on, we hence focus on RSR at the SiO₂/HfO₂ interface.

We can draw the main trends and identify the relevant structural parameters from semi-classical perturbation theory. Let $\Delta(\mathbf{r})$ and $\Delta'(\mathbf{r})$ be the SR profiles at the Si/SiO₂ and SiO₂/HfO₂ interfaces, and $\delta(\mathbf{r}) = \Delta'(\mathbf{r}) - \Delta(\mathbf{r})$ be the variations of the thickness of the IL. According to Fermi Golden Rule, the scattering rate between states $|\mathbf{k}\rangle$ and $|\mathbf{k}'\rangle$ with in-plane wave vectors $\mathbf{k}$ and $\mathbf{k}'$ is proportional to $|\langle \mathbf{k}' | H_R | \mathbf{k} \rangle|^2$, where H_R is the Hamiltonian of the SR + RSR disorder, the over-line denotes an average over configurations, and we have discarded band indexes for simplicity. This matrix element can be expanded in powers of Δ and δ

$$\langle \mathbf{k}' | H_R | \mathbf{k} \rangle = A(\mathbf{q})\Delta(\mathbf{q}) + B(\mathbf{q})\delta(\mathbf{q}) + \dots, \quad (1)$$

where $\mathbf{q} = \mathbf{k}' - \mathbf{k}$, $\Delta(\mathbf{q})$ and $\delta(\mathbf{q})$ are the Fourier transforms of $\Delta(\mathbf{r})$ and $\delta(\mathbf{r})$, and $A(\mathbf{q})$ and $B(\mathbf{q})$ are complex numbers. Hence, to second order in Δ and δ

$$\overline{|\langle \mathbf{k}' | H_R | \mathbf{k} \rangle|^2} = |A(\mathbf{q})|^2 \overline{|\Delta(\mathbf{q})|^2} + |B(\mathbf{q})|^2 \overline{|\delta(\mathbf{q})|^2} + A^*(\mathbf{q})B(\mathbf{q})\overline{\Delta^*(\mathbf{q})\delta(\mathbf{q})} + \text{c.c.} \quad (2)$$

The first term will be referred to as “pure SR” scattering (SR scattering is, indeed, usually computed^{15,16} with assumptions

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best compatible¹⁷ with $\delta=0$). It is proportional to $|\overline{\Delta(\mathbf{q})}|^2$, which is the Fourier transform of the auto-covariance function $F_\Delta(\mathbf{R}) = \overline{\Delta(\mathbf{r})\Delta(\mathbf{r}+\mathbf{R})}$ of the SR profile at the Si/SiO₂ interface ($\mathbf{r}$ and $\mathbf{R}$ being in-plane vectors). The second term is “uncorrelated” RSR scattering by fluctuations of the IL thickness. It is, likewise, proportional to the Fourier transform of the auto-covariance function $F_\delta(\mathbf{R}) = \overline{\delta(\mathbf{r})\delta(\mathbf{r}+\mathbf{R})}$ of these fluctuations.^{7–12} The third (and fourth complex conjugate) terms are “cross-correlated” contributions to RSR scattering. They are proportional to $\Delta^*(\mathbf{q})\delta(\mathbf{q})$, which is the Fourier transform of the correlation function $G(\mathbf{R}) = \overline{\Delta(\mathbf{r})\delta(\mathbf{r}+\mathbf{R})}$ between the SR profile at the Si/SiO₂ interface and the IL thickness fluctuations. They have not been accounted for in Refs. 7–12.

In general, one expects $|B(\mathbf{q})| \ll |A(\mathbf{q})|$, so that the cross-correlations prevail over the uncorrelated term unless $G(\mathbf{R}) \sim 0$ —which is unlikely in the thin ILs where RSR might be significant. The above analysis therefore shows that SR and RSR cannot be modeled as two independent mechanisms, as assumed in previous literature.

We consider an exponential (auto-)correlation model for the Si/SiO₂ interface profile $\Delta(\mathbf{r})$ and IL thickness variations $\delta(\mathbf{r})$ ¹⁵

$$\begin{aligned} F_\Delta(\mathbf{R}) &= \Delta^2 f(R); \quad F_\delta(\mathbf{R}) = \delta^2 f(R) \\ G(\mathbf{R}) &= \Delta \delta f(R)g, \end{aligned} \quad (3)$$

where $f(R) = e^{-\sqrt{2}R/L_c}$ and $L_c = 1.3$ nm everywhere. g characterizes the cross-correlations (or similarity) between $\Delta(\mathbf{r})$ and $\delta(\mathbf{r})$ ($|g| \leq 1$). This is equivalent to the following model for the SiO₂/HfO₂ interface profile $\Delta'(\mathbf{r})$:

$$\begin{aligned} F_{\Delta'}(\mathbf{R}) &= \overline{\Delta'(\mathbf{r})\Delta'(\mathbf{r}+\mathbf{R})} = \Delta'^2 f(R) \\ H(\mathbf{R}) &= \overline{\Delta(\mathbf{r})\Delta'(\mathbf{r}+\mathbf{R})} = \Delta \Delta' f(R)h, \end{aligned} \quad (4)$$

where $\Delta'^2 = \Delta^2 + \delta^2 + 2\Delta\delta g$ and $h = (\Delta + \delta g)/\Delta'$ is the overlap between the two interfaces. They are parallel if $h=1$, uncorrelated if $h=0$, and “anti-parallel” if $h=-1$ [Conversely, $\delta^2 = \Delta'^2 + \Delta^2 - 2\Delta\Delta'h$ and $g = (\Delta'h - \Delta)/\delta$]. Although the parameters Δ' and h are more intuitive,¹⁸ the equivalent (δ, g) set is more practical. Indeed, pure SR scattering simply corresponds to $\delta=0$; also, this set provides a straightforward criterion for the integrity of the SiO₂ layer: The surface covered by holes ($\delta(\mathbf{r}) < -t_{\text{IL}}$) in an IL with nominal thickness t_{IL} is $\lesssim 2.3\%$ as long as $\delta < t_{\text{IL}}/2$.¹⁹ The present results and conclusions might not, therefore, hold if $\delta \gg t_{\text{IL}}/2$.

The squared matrix element Eq. (2) thus reads

$$\begin{aligned} |\langle \mathbf{k}' | H_R | \mathbf{k} \rangle|^2 &= f(\mathbf{q}) \{ |A(\mathbf{q})|^2 \Delta^2 \\ &\quad + 2\text{Re}[A(\mathbf{q})B^*(\mathbf{q})] \Delta \delta g \}, \end{aligned} \quad (5)$$

where we have neglected the $\propto |B(\mathbf{q})|^2 \delta^2$ term.

Finally, let μ_{SR} be the SR-only mobility (computed for strictly parallel interfaces,¹⁷ i.e., $\delta=0$) and $\mu_{\text{SR+RSR}}$ the total SR + RSR mobility. Let us define the RSR mobility as $\mu_{\text{RSR}}^{-1} = \mu_{\text{SR+RSR}}^{-1} - \mu_{\text{SR}}^{-1}$. Then, we expect from Eq. (5) in a semi-classical Kubo-Greenwood approach

$$\mu_{\text{RSR}}^{-1} \simeq -C_{\text{RSR}}^{-1} \Delta \delta g, \quad (6)$$

where C_{RSR} is a constant. The RSR mobility is therefore inversely proportional to the rms fluctuations Δ and δ , and to the overlap g . Note that μ_{RSR} (as defined above) can be positive or negative, i.e., remote surface roughness can either enhance or inhibit the flow of carriers depending on g . We will discuss the underlying physics later.

In order to verify these assertions, we have performed NEGF calculations of the mobility in *n*FDSOI devices along the lines of Ref. 13 (same structures). We have considered $t_{\text{Si}} = 4$ and $t_{\text{Si}} = 8$ nm thick (001) Si films (dielectric constant $\epsilon_{\text{Si}} = 11.7$) on a 25 nm thick buried oxide and a grounded *n*-doped Si substrate. The front gate stack is made of an IL of SiO₂ with varying thickness t_{IL} ($\epsilon_{\text{IL}} = 3.9$), a 2.4 nm thick layer of HfO₂ ($\epsilon_{\text{HfO}_2} = 22$), and a metal gate. We use the effective mass approximation for electrons. The wave functions can penetrate in the IL. Electron-phonon (PH) interactions are included in all calculations, but cancel out in μ_{RSR} (see Ref. 13 for the methodology and a discussion about Matthiessen’s rule).

The advantage of NEGF is that it makes use of an explicit, real space description of SR/RSR disorders, and screening (no need for an approximation to the very complex H_R as in Kubo-Greenwood calculations). This allows for accurate calculations of SR mobilities.¹³ In the present case, we have computed mobilities in samples of SR/RSR disorder satisfying Eq. (3) (see Fig. 1), and averaged over a few configurations until convergence.

As an illustration, the total SR + RSR mobility $\mu_{\text{SR+RSR}}^{-1} \equiv \mu_{\text{SR}}^{-1} + \mu_{\text{RSR}}^{-1}$ is plotted as a function of carrier density n and g in Fig. 2(a), and as a function of δ and g in Fig. 2(b). As expected from Eq. (6), $\mu_{\text{SR+RSR}}^{-1}$ is pretty linear with δ and g , and does not show, in particular, very significant $\propto \delta^2$ contributions from the uncorrelated term in Eq. (2). We have also checked that RSR at the HfO₂/Metal gate interface had much less impact on the mobility, at least for the HfO₂ thickness ≥ 2 nm considered here.

The RSR mobility computed for $g = -1$ is plotted as a function of carrier density for different film and IL thicknesses in Fig. 3. Since $\mu_{\text{RSR}} > 0$ when $g < 0$, the total mobility decreases when the fluctuations of the IL thickness are

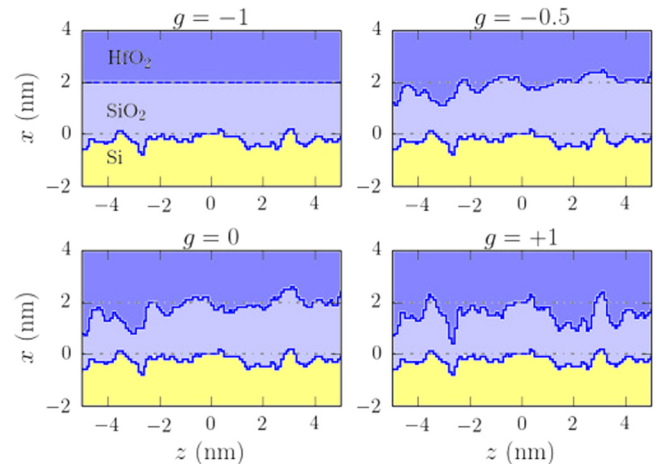


FIG. 1. Surface roughness profiles computed for different g 's ($\Delta = \delta = 0.47$ nm and $t_{\text{IL}} = 2$ nm). Note that the SiO₂/HfO₂ interface is actually smooth when $\Delta = \delta$ and $g = -1$. The $g = -0.5$ stack approximately lies on the curve “ $\Delta' = 0.47$ nm and $\lambda = 2.6$ nm” of Fig. 4.

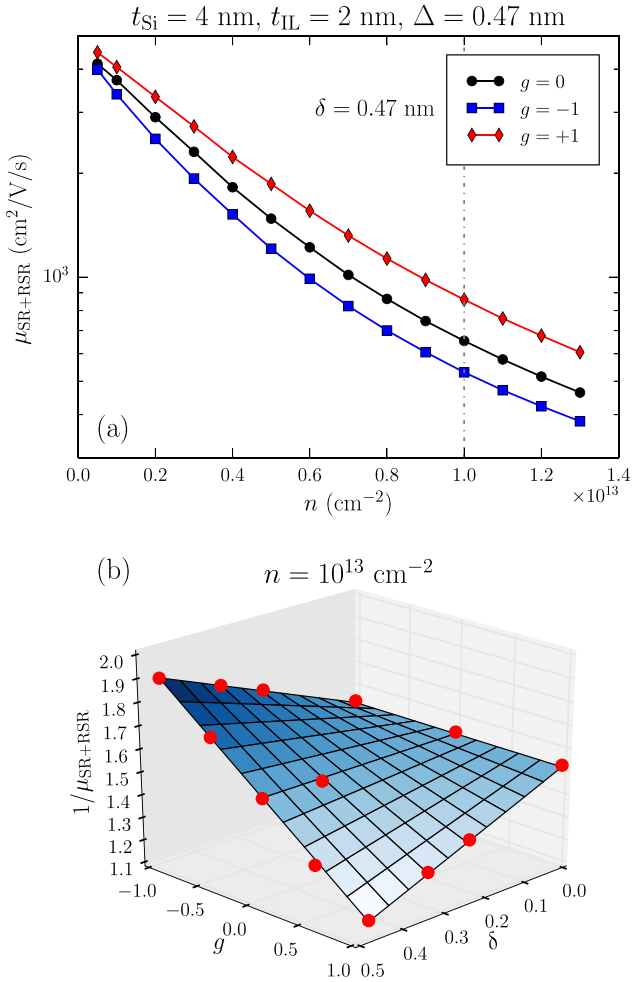


FIG. 2. (a) $\mu_{\text{SR}+\text{RSR}}$ as a function of carrier density n and g in an n FDSOI device with $t_{\text{Si}} = 4$ nm and $t_{\text{IL}} = 2$ nm ($\Delta = \delta = 0.47$ nm) (b) $\mu_{\text{SR}+\text{RSR}}^{-1}$ (10^{-3} V s/cm²) as a function of δ (nm) and g in the same device, at $n = 10^{13}$ cm⁻². The red dots are the NEGF data, the blue surface is the best fit $\mu_{\text{SR}+\text{RSR}}^{-1} \equiv \mu_{\text{SR}}^{-1} + C_{\text{RSR}}^{-1} \Delta \delta g$.

anti-correlated to the SR profile. Indeed, the carriers, squeezed by the surface electric field F_s , tend to localize where $\Delta(\mathbf{r}) > 0$; localization and scattering are enhanced by

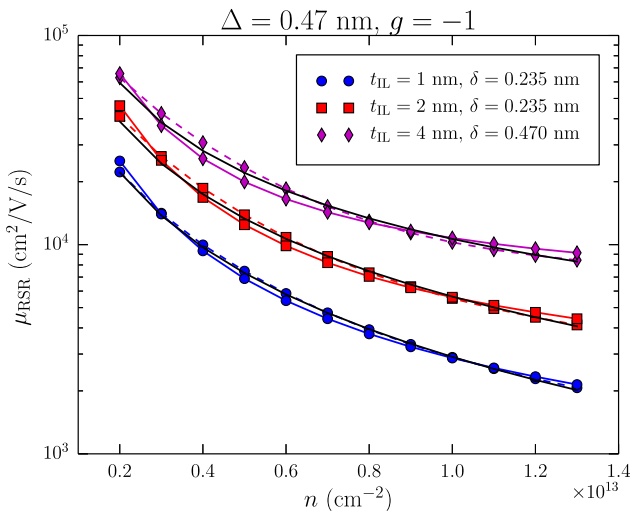


FIG. 3. RSR mobilities in 4 nm thick (dashed color lines with symbols) and 8 nm thick (solid color lines with symbols) Si films with $\Delta = 0.47$ nm and $g = -1$. Black lines are Eqs. (6) and (7).

the concomitant increase of F_s when $g < 0$ (IL tends to thin where $\Delta(\mathbf{r}) > 0$), and are, conversely, inhibited by the concomitant decrease of F_s when $g > 0$ (IL tends to thicken where $\Delta(\mathbf{r}) > 0$). As expected, the RSR mobility decreases with increasing carrier density (or equivalently F_s) as the carriers move closer to the top gate stack; hence RSR is most efficient (as is surface roughness) in the strong inversion regime, at variance with RCS, for example. As such, it is weakly dependent on the thickness of the silicon film in the investigated range $t_{\text{Si}} \geq 4$ nm. It shows, though, a strong (exponential) dependence on the thickness of the IL; the thinner the IL the stronger the RSR correction.

From these calculations, we can extract the prefactor $C_{\text{RSR}}(n, t_{\text{IL}})$ as a function of the carrier density n and thickness of the IL. The Fourier components of the electric field suggest^{7,12} that $C_{\text{RSR}}^{-1} \sim K e^{-\alpha t_{\text{IL}}}$. Expanding K and α in powers of n , we tentatively fit the NEGF data with

$$C_{\text{RSR}}^{-1} = a n \left(1 + \frac{n}{n_1} \right) \exp \left[- \left(1 + \frac{n}{n_2} \right) \frac{t_{\text{IL}}}{t_0} \right], \quad (7)$$

and get $a = 2.96 \times 10^{-2}$ V s/cm², $n_1 = 9.6 \times 10^{12}$ cm⁻², $t_0 = 1.87$ nm, and $n_2 = 4.1 \times 10^{13}$ cm⁻². Equation (7) reproduces the NEGF data very well for $n > 2 \times 10^{12}$ cm⁻², as shown on Fig. 3.

How large can RSR scattering be in actual devices? As an illustration, we make the following assumption for the correlations between the Si/SiO₂ and SiO₂/HfO₂ interfaces:¹⁸

$$h(t_{\text{IL}}) = e^{-t_{\text{IL}}/\lambda}, \quad (8)$$

where λ is a vertical correlation length. The total PH + SR + RSR + RCS mobility is plotted a function of t_{IL} in Fig. 4, for a 8 nm thick film in the strong inversion regime, and for different λ and Δ' . RCS was modeled as a distribution of positive charges at the SiO₂/HfO₂ interface^{13,14} with density

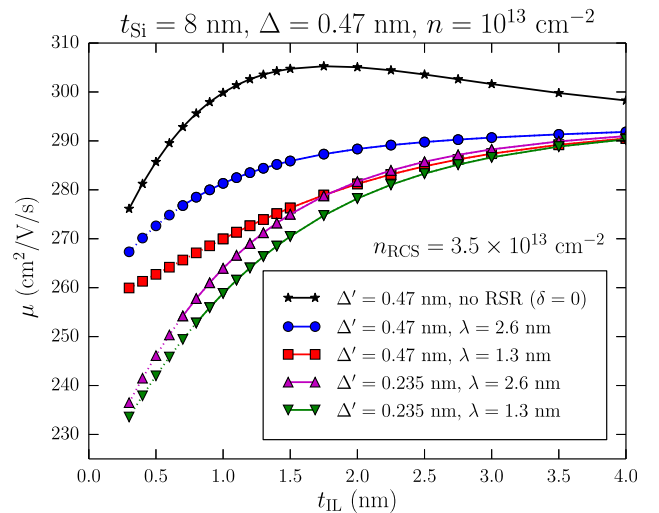


FIG. 4. Total mobility (PH + SR + RSR + RCS) in a 8 nm thick n FDSOI film as a function of t_{IL} , for different rms roughness Δ' at the SiO₂/HfO₂ interface, and for different vertical correlation lengths λ [Eq. (8)] ($\Delta = 0.47$ nm and $n_{\text{RCS}} = 3.5 \times 10^{13}$ cm⁻²). The carrier density is $n = 10^{13}$ cm⁻² (effective field $E_{\text{eff}} \sim 0.8$ MV/cm). The data were interpolated from a set of NEGF calculations. The lines are dotted wherever $\delta > t_{\text{IL}}/2$, i.e., when the IL might be pierced in many places.

$n_{\text{RCS}} = 3.5 \times 10^{13} \text{ cm}^{-2}$. In the absence of RSR, the mobility is weakly dependent on the IL thickness, at variance with experimental data.²⁰ The RSR can, however, significantly enhance scattering in thin ILs. It is, notably, very detrimental if the $\text{SiO}_2/\text{HfO}_2$ interface is smoother than the Si/SiO_2 interface, because the IL thickness fluctuations become anti-correlated to the Si/SiO_2 roughness profile ($\delta \rightarrow \Delta$ and $g \rightarrow -1$ when $\Delta' \rightarrow 0$). Note that alloying SiO_2 with HfO_2 near the IL/High- κ interface might blur the variations of the dielectric constant and effectively smooth that interface. A more detailed comparison with experiment²⁰ would call for a comprehensive de-embedding of the different scattering mechanisms.¹⁴ Yet we can conclude that RSR, together with RPH^{5,6} (not accounted for at present in NEGF), are serious candidates in explaining the trends measured in very thin IL devices at strong inversion.

Finally, we would like to discuss the effects of non-parabolic (NP) corrections and exchange-correlation (XC) effects. NP corrections can be included using a two bands $\mathbf{k} \cdot \mathbf{p}$ model^{13,21} for the conduction band, yet at a much larger numerical cost. Long-range XC effects have been modeled by an image charge self-energy correction (numerically computed along the lines of Ref. 22), and short-range XC effects by a local density approximation.^{16,23} Calculations on a few representative configurations show that NP and XC corrections both decrease the mobility and C_{RSR} (i.e., enhance RSR scattering), by a total of $\sim 20\%$.

To conclude, we have discussed the impact of remote surface roughness scattering (RSR) at the $\text{SiO}_2/\text{HfO}_2$ interface on the electron mobility in FDSOI thin films. We show that the RSR corrections are dominated by the cross-correlations between the two interfaces of the IL. The mobility increases when the SiO_2 thickness fluctuations are correlated with those of the Si/SiO_2 interface, and decreases otherwise. SR and RSR cannot, therefore, be described as two independent mechanisms, and must be modeled concurrently. The RSR mobility shows an exponential dependence on the IL thickness. In particular, RSR might be significant at strong inversion in thin IL devices, where the $\text{SiO}_2/\text{HfO}_2$ interface is (dielectrically) smoother than the Si/SiO_2 interface.

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