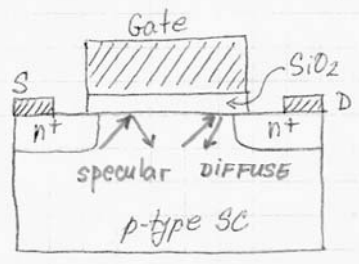### (B) SURFACE - ROUGHNESS SCATTERING

- Confined carriers at the Si-SiO_2 interface are subject to all the scattering mechanisms that affect 3D carriers, but some additional mechanisms also occur. The most important one is that the carriers can scatter off the boundaries of the confining potential. Since the gate is at fixed potential, any fluctuations in the oxide thickness will produce fluctuations in the confining potential, and therefore, on the energy level spectrum in the triangular potential well. The effect increases when the applied voltage on the gate increases, because carriers are confined more closely to the interface.

(a) low gate biases (low N_s) coulomb scattering due to ionized acceptors in the depletion region dominates

(B) High gate biases: Coulomb scattering less important because of large screening (large N_s). Surface-roughness dominates due to the closer confinement of the carriers to the interface.

- To evaluate scattering due to surface roughness, we need to identify the perturbing potential. Let $V(z')$ be the confining potential along the growth direction, where:

$$z' = z + \Delta(\vec{r})$$

position of the point without interface roughness

random function that describes deviations from the atomically flat interface.

Using Taylor-series expansion, we get:

$$V(z + \Delta(\vec{r})) = V(z) + \frac{\partial V}{\partial z} \Delta(\vec{r}) = V(z) + e \mathcal{E}_z(z) \cdot \Delta(\vec{r}) + \cdots$$

Therefore, the perturbing potential is given by:

$$H_{SR} = e\,\mathcal{E}_z(z) \cdot \Delta(\vec{r})$$

where $\mathcal{E}_z(z)$ is the electric field along the confining direction.

• The matrix element for scattering between states $\vec{k}_{\shortparallel}$ and $\vec{k}_{\shortparallel}{}'$ in subbands n and m is then given by:

$$M(\vec{k}_{\shortparallel}, \vec{k}_{\shortparallel}{}')_{nm} = e\underbrace{\int \psi_m^*(z)\,\mathcal{E}_z(z)\,\psi_n(z)\,dz}_{} \times \frac{1}{A}\int e^{\,i(\vec{k}_{\shortparallel} - \vec{k}_{\shortparallel}{}')\cdot \vec{r}_1}\,\Delta(\vec{r}_1)\,d^2r_1$$

Weighted average of the electric field along the confining direction (F_{nm})

Therefore:

$$|M(\vec{k}_{\shortparallel}, \vec{k}_{\shortparallel}{}')|^2_{nm} = e^2\,|F_{nm}|^2 \times \frac{1}{A}\int d^2r_1\, e^{-i(\vec{k}_{\shortparallel} - \vec{k}_{\shortparallel}{}')\cdot \vec{r}_1}\,\Delta(\vec{r}_1) \times \frac{1}{A}\int d^2r_2\, e^{\,i(\vec{k}_{\shortparallel} - \vec{k}_{\shortparallel}{}')\cdot \vec{r}_2}\,\Delta(\vec{r}_2)$$

$$= e^2\,|F_{nm}|^2\,\frac{1}{A^2}\int d^2r_1 \int d^2r_2\, e^{\,i(\vec{k}_{\shortparallel} - \vec{k}_{\shortparallel}{}')\cdot(\vec{r}_2 - \vec{r}_1)}\,\underbrace{\Delta(\vec{r}_2)\,\Delta^*(\vec{r}_1)}_{}$$

random variables

The expectation value of $|M(\vec{k}_{\shortparallel}, \vec{k}_{\shortparallel}{}')|^2_{nm}$ over many samples leads to:

$$\langle|M(\vec{k}_{\shortparallel}, \vec{k}_{\shortparallel}{}')|^2_{nm}\rangle = e^2\,|F_{nm}|^2\,\frac{1}{A^2}\int d^2r_1 \int d^2r_2\, e^{\,i(\vec{k}_{\shortparallel} - \vec{k}_{\shortparallel}{}')\cdot(\vec{r}_2 - \vec{r}_1)}\,\langle\Delta(\vec{r}_2)\,\Delta^*(\vec{r}_1)\rangle$$

The correlation between $\Delta^*(\vec{r}_1)$ and $\Delta(\vec{r}_2)$ is measured by the joint momenta, i.e.

$$R(\vec{r}_1, \vec{r}_2) = \int d^2r_1 \int d^2r_2\; \Delta^*(\vec{r}_1)\,\Delta^*(\vec{r}_2)\,\underbrace{P[\Delta(\vec{r}_1), \Delta(\vec{r}_2)]}_{}$$

joint probability density

When the process is stationary, the autocorrelation function $R(\vec{r}_1, \vec{r}_2)$ depends only upon the difference $\vec{r}_1 - \vec{r}_2$. In this case:

$$R(\vec{r}_1, \vec{r}_2) = \langle\Delta(\vec{r}_2)\,\Delta^*(\vec{r}_1)\rangle = R(\vec{r}_1 - \vec{r}_2)$$

and:

$$\langle |H(\vec{k}_{\shortparallel},\vec{k}_{\shortparallel}')|^2_{nm} \rangle = e^2|F_{nm}|^2 \frac{1}{A^2} \int d^2\vec{r}_1 \int d^2 r_2\, e^{-i(\vec{k}_{\shortparallel}-\vec{k}_{\shortparallel}')\cdot(\vec{r}_1-\vec{r}_2)}\, R(\vec{r}_1-\vec{r}_2)$$

$$= e^2|F_{nm}|^2 \frac{1}{A^2} \int d^2 r_1 \int d^2 r\, e^{-i(\vec{k}_{\shortparallel}-\vec{k}_{\shortparallel}')\cdot\vec{r}}\, R(\vec{r})$$

where we have introduced $\vec{r} = \vec{r}_1 - \vec{r}_2$ and we have replaced the integration with respect to r_2 with an integration with respect to $\vec{r}$. The spectral characteristics of the stochastic process are obtained by computing the Fourier transform of the autocorrelation function $R(\vec{r})$. This gives the distribution of power with frequency, i.e.

$$S(\vec{q}_{\shortparallel}) = \int d^2 r\, e^{-i\vec{q}_{\shortparallel}\cdot\vec{r}}\, R(\vec{r}) \quad, \quad \text{where } \vec{q}_{\shortparallel} = \vec{k}_{\shortparallel} - \vec{k}_{\shortparallel}'$$

The quantity $S(\vec{q}_{\shortparallel})$ is, thus, called power spectral density. To summarize:

$$\langle |H(\vec{k}_{\shortparallel},\vec{k}_{\shortparallel}')|^2_{nm} \rangle = e^2|F_{nm}|^2 \frac{1}{A^2} \int d^2 r_1\, S(\vec{q}_{\shortparallel}) = e^2|F_{nm}|^2 \frac{S(\vec{q}_{\shortparallel})}{A}$$

- The autocorrelation function $R(\vec{r})$ is usually assumed to be exponential function, i.e.

$$\langle \Delta^*(\vec{r}_1)\, \Delta(\vec{r}_2) \rangle = R(\vec{r}_1 - \vec{r}_2) = R(\vec{r}) = \Delta^2 e^{-r/L}$$

where Δ is the rms amplitude of the fluctuations and L is their correlation length (roughly the distance between fluctuations). Typical values are:

$$\Delta \approx 2 - 4\,\text{Å}$$
$$L \approx 10 - 30\,\text{Å}$$

The power spectrum of $R(\vec{r})$ is then given by:

$$S(\vec{q}_{\shortparallel}) = \bar{u}\,\Delta^2 L^2 \frac{1}{1 + \frac{1}{2}L^2 q_{\shortparallel}^2}$$

To summarize, the probability for transition per unit time between states $\vec{k}_{\shortparallel}$ and $\vec{k}_{\shortparallel}'$ is given by:

$$S(\vec{k}_{\shortparallel}, \vec{k}_{\shortparallel}') = \frac{2\bar{u}}{\hbar} e^2 |F_{nm}|^2 \; \frac{S(\vec{q}_{\shortparallel})}{A} \; \delta(E' - E)$$

final state energy ↗   ↖ initial state energy

i.e.

$$S(\vec{k}_{\shortparallel}, \vec{k}_{\shortparallel}') = \frac{2\bar{u}}{\hbar} e^2 |F_{nm}|^2 \; \frac{1}{A} \bar{u}\Delta^2 L^2 \; \frac{1}{1 + \frac{1}{2} L^2 q_{\shortparallel}^2} \; \delta(E' - E)$$

The initial and final state energies are given by:

$$\begin{cases} E = E_n + \dfrac{\hbar^2 k_{\shortparallel}^2}{2m^*} \\[2mm] E' = E_m + \dfrac{\hbar^2 k_{\shortparallel}'^2}{2m^*} \end{cases}$$

• Note on the strength of the scattering process:

Surface-roughness is affected by both Δ and F_{nm}. Δ is the measure of the roughness of the interface and F_{nm} in a way is a measure how close (on the average) are the carriers from the Si/SiO_2 interface.