SO phonon scattering rates at the Si-HfO₂ interface in Si MOSFETs

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Abstract. Silicon MOSFETs with high κ gate stacks offer a significant reduction in gate leakage current, but the presence of soft surface optic phonon modes degrades the mobility. A progressively more complex set of models for SO phonon scattering at the Si-HfO₂ interface is presented based upon dynamic screening models. Landau damping of the electron-phonon-plasmon coupling is examined by simple approximations. A novel approach to determining the re-normalised phonon spectrum based on Padé approximants is outlined as a route to obtaining practical scattering rate for Monte Carlo simulation.

1. Introduction

The recent trend to high-κ dielectric gate stack MOSFETs has been driven by the requirement to reduce gate leakage due to tunnelling through the insulator that bedevils the ultra-thin silicon dioxide required for sub 45 nm devices. The introduction of a high-κ dielectric such as HfO₂ leads to the same gate capacitance for a thicker oxide layer given by

\[ t_{\text{high}} = \frac{\kappa_{\text{high}}}{\kappa_{\text{ox}}} t_{\text{SiO}_2} \]  

Unfortunately, a severe mobility degradation ensues because of the strong coupling of carriers in the channel to surface soft optical (SO) phonons in the vicinity of the dielectric interface. The SO modes are easily excited at room temperature and lead to strong mobility reduction. A precise valuation of SO scattering has proved elusive because of the complexity of the dynamically screened coupling between plasmons in the gate and channel and the oxide phonons. Here we report progress towards a practical evaluation of the scattering rate due to SO phonon interactions in high-κ dielectric MOSFETs. The objective is to provide input for ensemble Monte Carlo simulation codes.

2. Bulk simulations

The trend to mobility degradation in different material systems may be seen in the simulation results of our Monte Carlo simulation shown in Figure 1. In figure 1(a) the effective mobility is computed for silicon and strained silicon and compared with bulk silicon with the same equivalent oxide thickness (EOT). Figure 1(b) compares the predicted and experimental mobility versus oxide interfacial layer thickness with a constant inversion layer field of 1000kV/cm. In these bulk simulations only a very primitive model is used for the SO phonon scattering: each material is treated as homogeneous and no Landau damping of the coupled plasmon-phonon-electron system is incorporated. For device modeling it is crucial to develop better approximations that capture the essentially inhomogeneous nature of the coupled gate, dielectric layers and channel. The
inhomogeneities arise because of the variation in electron density and temperature along the channel of a MOSFET and because realistic gate stacks display phase separation and polycrystallinity effects.

Figure 1. (a) Computed effective electron mobilities for bulk Si and strained Si, with SiO$_2$, and bulk Si with EOT HfO$_2$ dielectric, assuming the same geometrical interface roughness description as for SiO$_2$.

(b) Comparison between computed and experimental mobility versus oxide interfacial layer thickness with a constant inversion layer field of 1000kV/cm.

### 3. 25 nm MOSFET simulation

Figure 3 (a) shows the layout of a $n$-MOSFET, with a gate length $L_G = 25$nm and equivalent oxide thicknesses (EOT) = 0.9nm, suitable for a high-performance MOSFET belonging to the 65nm technology node. In Figure 3 (b) we show the corresponding computed $I_{DS}$-$V_{DS}$ device characteristics for high $V_{SD} = 1.0V$ with and without the impact of SO phonon scattering. The underlying homogeneous model is based upon the following. The important scattering mechanism is between electrons in the channel and quasi-particles originating from the plasmon (Gate and Substrate)-phonon coupling: in thin-insulator structures, this coupling affects significantly the interaction between the excitations at the interface and the electrons in the channel, therefore the gate stack can no longer be treated as independent regions of metal or poly-Si, oxide and substrate. The surface potential is computed by solving the Poisson-Helmholtz equation across the different layers/interfaces. Following the methodology of Fischetti et al $[3]$ the resulting dispersion relation takes the form:

$$
\varepsilon_{hk}^2(\omega) + \varepsilon_{ad}(\omega) \left\{ \varepsilon_{gate}(\omega) + \varepsilon_{ad}(\omega) \right\} \text{Cotb}\left[ Q_{hk} \right] + \varepsilon_{gate}(\omega)\varepsilon_{ad}(\omega) = 0; \quad \omega = \omega(Q)^j, j = 1...6
$$

(2)

where for the high-$\kappa$ layer, gate and silicon channel plasmon dielectric responses we choose:

$$
\varepsilon_{gate}(\omega) = \varepsilon_{gate}^{\omega} \left( 1 - \frac{\omega^2}{\omega_p^2} \right) ; \quad \varepsilon_{ad}(\omega) = \varepsilon_{ad}^{\omega} \left( \frac{\omega_1^2 - \omega^2}{\omega_1^2 - \omega_2^2} \right) \frac{\omega_1}{\omega_1^2 - \omega^2} \quad ; \quad \varepsilon_{ad}(\omega) = \varepsilon_{Si}^{\omega} \left( 1 - \frac{\omega_p^2}{\omega^2} \right).
$$

(3)

The dispersion relation (2) is a 6th order polynomial in $\omega^2$. There are 6 positive modes arising from the coupling; 2 TO like modes in the dielectric layer, 4 surface modes (groups of 2 modes localized near each of the 2 interfaces) representing coupled-interface-phonon plasmon modes. Figure 4 (a) shows the scattering rates for the dominant processes in the zero damping plasmon-pole approximation.
4. Modelling the coupled plasmon-phonon in realistic systems

In realistic high-κ MOSFETs, the gate stack comprises an interfacial SiO$_2$ layer (thickness $t_{ox}$), a main HfO$_2$ layer (thickness $t_{hk}$) and a metallic gate layer. The actual dielectric response cannot be homogeneous because the electron concentration and electron temperature vary along the device channel thus altering the plasmon energy and Landau damping. This problem is highly complicated and we look for simplifications. In a small region (cell) of the model device the surface potential may be computed as in section 3, the resulting dispersion relation is a 16th order polynomial in $\omega^2$.

\[
\frac{\epsilon_{gate} + \epsilon_{hk}}{\epsilon_{Si} + \epsilon_{ox}}(\epsilon_{Si} + \epsilon_{ox})(\epsilon_{ox} - \epsilon_{hk}) \exp[-2Q(t_{hk} + t_{ox})] - (\epsilon_{gate} - \epsilon_{hk})(\epsilon_{Si} - \epsilon_{ox})(\epsilon_{ox} - \epsilon_{hk}) \exp[-2Q(t_{hk} + t_{ox})] = 0
\]  

(4)

There are 16 different positive modes arising from the coupling; 2 TO like modes in each dielectric layer, 12 surface modes (groups of 4 modes localized near each of the 3 interfaces). If we include the variation in plasma frequency throughout the channel, the presence of high Q events and the variation of electron temperature in the strong driving fields, the evaluation of a position dependent scattering rate becomes problematic. To incorporate the additional processes it is necessary to invoke the Lindhard dielectric function for the channel and gate responses. The Lindhard function handles all wavevectors, finite temperatures and Landau damping. For non-degenerate carriers it yields

\[
\varepsilon(Q, \omega) = \varepsilon_{Si} - \frac{e^2 m^*}{4\pi^{3/2} h^2 Q^3} \left( \frac{2m^* k_B T_e}{\hbar^2} \right)^{-1} e^{Re \mu} \{Z^+(W) - Z^-(W)\}
\]

(5)

\[
Z(z) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp[-u^2] \, du; \quad W_\pm = \left( \frac{2m^* k_B T_e}{\hbar^2} \right)^{-1} \left( \frac{m^* \omega}{\hbar Q} \pm \frac{Q}{2} + i\eta \right)
\]

(6)

Here $Z$ is the plasma dispersion function. The complexity of (5) and (6) makes finding the modes intractable. But as a first step forward, the Landau damping may be incorporated crudely by cutting off the coupling to the gate and channel plasmons when the wave vector $Q$ is sufficiently large that the plasmon like modes enter the single particle excitation regime. The dispersions are shown in Fig.4 (b).

5. Landau damping: a new simplified but accurate approach

In order to completely treat the Lindhard function and at the same time resort to solving a polynomial dispersion relations for the modes we recall a Padé approximant for $Z$ introduced before [7].

\[
Z(z) = \frac{i\sqrt{\pi} + (\pi - 2)z}{1 - i\sqrt{\pi}z - (\pi - 2)z^2}
\]

(7)
Expression (7) is a ratio of low order polynomials in frequency $\omega$. It leads to a tractable dispersion relation including Landau damping. The accuracy of the approximant is shown in Fig.5 (b).

Figure 5 (a) shows the kernel of the channel dielectric response (5) $F(Q,\omega) = \{Z(W^+) - Z(W^-)\}$ as a function of $\varepsilon(Q)/\hbar\omega = (\hbar^2 Q^2 / 2m^*)/\hbar\omega$ and electron temperature. The Landau damping regime is clear. In this form it is possible to gain analytical solutions to the plasmon-phonon dispersion relations and to the phonon and plasmon content of the various modes.

6. Conclusion

A simplified Landau damping has been introduced for modeling of complex high-$\kappa$ gate stacks. It permits analytical evaluation of re-normalised phonon and plasmon energies and scattering rates, especially for inhomogeneous layers. With appropriate modifications to the channel polar optic phonon interaction, the formalism is extendable to III-V based MOSFETs.

References

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