Model Plasma Dispersion Functions for SO Phonon Scattering in Monte Carlo Simulations of High-κ Dielectric MOSFETs

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The recent interest in high-κ dielectric MOSFETs to overcome gate leakage problems has raised a number of problems for accurate Monte Carlo based device simulation of such devices. The problem is caused by carrier scattering on soft surface optic (SO) phonons. It leads to a strong degradation of effective mobility. A precise quantification of the mobility degradation requires us to compute the electron-phonon scattering rates as a function of position within the channel, the dependence on local carrier concentration n and carrier temperature T_e, the gate stack layer thickness variations and inhomogeneities within the dielectric regions. The situation is exacerbated by the role of plasmons in the channel and gate regions [1]. The core problem for implementing Monte Carlo simulation with SO phonon scattering is the development of fast algorithms for the dynamically-screened position-dependent scattering rates. Unfortunately, the re-normalised coupling of the phonons and plasmons is sensitive to the gate stack inhomogeneities and the variation in $n(\mathbf{r})$ and $T_e(\mathbf{r})$ along the channel. In the present work we significantly extend earlier studies [1] that utilised the simple plasmon-pole approximation for the electronic dielectric functions $\varepsilon(q,\omega)$ in the gate and channel plasmas. We proceed by evaluating the Lindhard function for the gate and channel carrier assemblies so as to include dynamic screening and Landau damping. For example in the Si channel,

$$\varepsilon_e(q,\omega) = \varepsilon_{Si} - \frac{e^2 m^{2} * k_B T_e}{2\pi^{3/2}\hbar^3 q^3}\{Z(W^+) - Z(W^-)\} \qquad (1)$$

At the heart of the calculation is the plasma dispersion function Z, that depends upon the energy distribution function f_0 which is Maxwell-Boltzmann for non-degenerate systems and Fermi-Dirac for degenerate systems.

$$Z(z) = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{f_0(u^2)}{u-z}du;\ (u^2 \equiv E/k_B T_e) \qquad (2)$$

(2)

$$W_{\pm} = \left(\frac{2m^* k_B T_e}{\hbar^2}\right)^{-1/2}\left(\frac{m^*\omega}{\hbar q} \pm \frac{q}{2} + i\eta\right). \qquad (3)$$

In principle the scattering-out rate $\lambda(\mathbf{k})$ at a position $\mathbf{r}$ may be expressed in the Born approximation in terms of an angular frequency integral over the complex dielectric permittivity:

$$\lambda(\mathbf{k}) = \int_{-\infty}^{\infty} d(\hbar\omega)\pi^{-1}\{1 + f_{BE}(\omega)\}$$
$$\sum_{\mathbf{q}}\{1 - f(\mathbf{k}+\mathbf{q})\}\ \frac{2\pi}{\hbar}|V(\mathbf{q})|^2\ \mathrm{Im}\{-\frac{1}{\varepsilon(q,\omega)}\}$$
$$\delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \hbar\omega). \qquad (4)$$

In the present paper we present new analytical models for the non-degenerate and degenerate plasma dispersion functions Z based on rational fractions of low order polynomials in angular frequency ω. With such a formulation the problem of computing the re-normalised phonon and plasmon energies together with scattering strengths as functions of wave vector is considerably simplified. Figures (1-3) compare the analytical approximations with direct numerical computation of the dispersion functions. A second new development reported here is the evaluation of the final scattering state from (4) using importance sampling with applications to realistic MOSFETs.

References

[1] M.V. Fischetti, D. A. Neumayer and E. A. Cartier, J. App. Phys. **90**,4587-4607 (2001).

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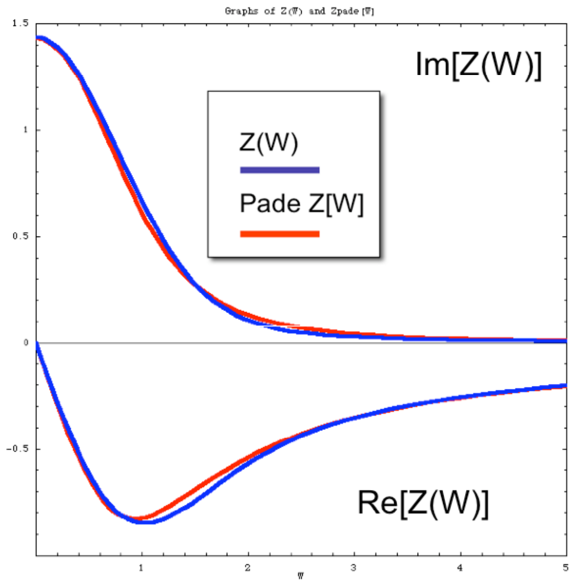

Fig. 1. The real and imaginary part of the dispersion function Z for non- degenerate systems with $T = 300K,$ and zero collisional damping . The figure compares the numerically computed result Z(W) with the analytical Padé approximant model.

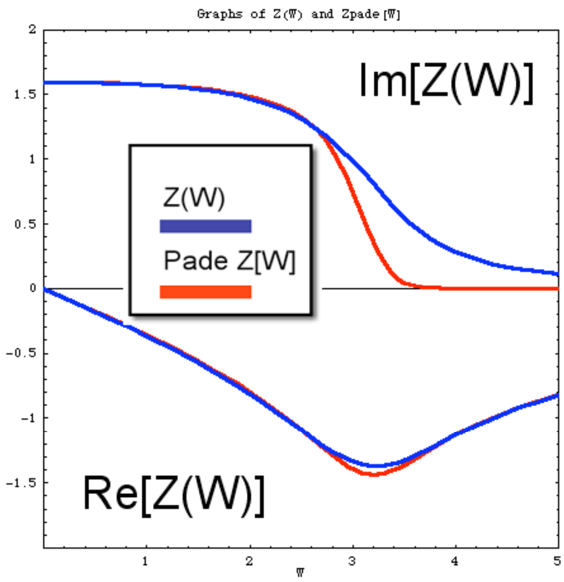

Fig. 2. The real and imaginary part of the dispersion function Z for strongly collision damped degenerate systems with $\varepsilon_F - \varepsilon_c = 10 \ \ k_B T; \ T = 300K,$ and damping factor $\Gamma / k_B T = 0.25$.

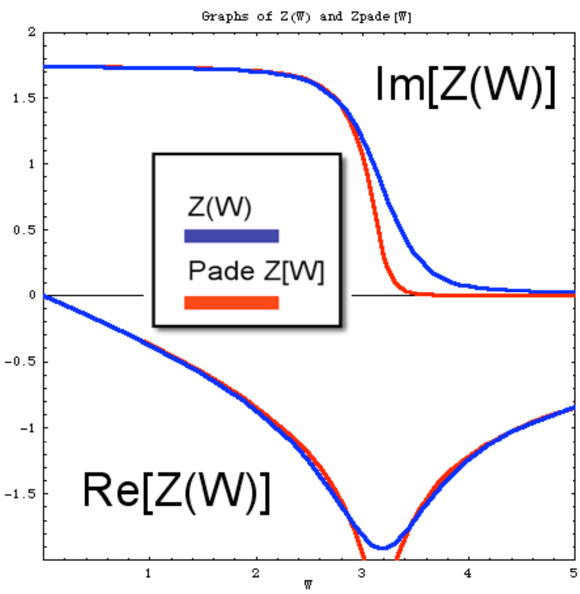

Fig. 3. The real and imaginary part of the dispersion function Z for weakly collision damped degenerate systems with $\varepsilon_F - \varepsilon_c = 10 \ \ k_B T; \ T = 300K,$ and damping factor $\Gamma / k_B T = 0.01$.