A New Microscopic Formalism for the Electron Scattering by Remote "Paired" Dipoles in HKMG MOSFETs

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Abstract

We devise a new microscopic formalism for the remote dipole scattering (RDS) limited relaxation time in the inversion layers of HKMG MOSFETs. This formalism can apply to two different dipole configurations: (i) a "one dipole" configuration and (ii) a "paired dipoles" configuration. We find that when fitting the inversion-layer effective electron mobility measured from the industry-level hafnium-based metal gate MOSFETs, the former configuration yields a large value of the HK/IL interface dipole density of around 10^{15} cm^{-2}, accompanied by a large threshold voltage shift ΔV_{th_dipole} of 12 V. These values are comparable with those of the existing Monte Carlo simulation. More importantly, in case of the latter configuration (paired dipoles) plus the experimentally determined fixed charges, the corresponding values can be significantly reduced to 10^{14} cm^{-2} and 2 V, which are quite close to the experimental estimations in the literature.

Introduction

Obvious mobility degradation has been observed due to the application of HKMG stack in MOSFETs [1]. Fixed charges in the gate stack may be responsible via remote Coulomb scattering (RCS) [2]. However, the extracted fixed charges density is unreasonably large in magnitude. Alternatively, the dipoles specific to HKMG stack have an influence on the threshold voltage [3], along with the density of typical 10^{14} cm^{-2} as demonstrated from the experiment [3] and the *ab initio* calculation [4].

Indeed, the importance of the remote Coulomb dipoles (RDS) as the intrinsic origin of the inversion-layer mobility degradation of HKMG MOSFETs has been experimentally highlighted [5]. To provide a deeper understanding of the dipoles involved, sophisticated device simulation is indispensable. Monte Carlo simulation task [6] has been performed in this direction; however, the dipole density thus extracted from the HKMG mobility data still delivered a value of 10^{15} cm^{-2}, which is tenfold larger than that of *ab initio* [4] and thereby leads to threshold voltage shift ΔV_{th_dipole} as large as 10 V.

To suppress such large values, in this paper, we propose a new physical origin in terms of the "paired dipoles" configuration, followed by a microscopic inversion-layer electron mobility simulation and its experimental extraction task.

Experimental Task

The experimental sample is the industrial hafnium-based metal gate silicon bulk n-channel MOSFETs. The gate length is 910 nm.

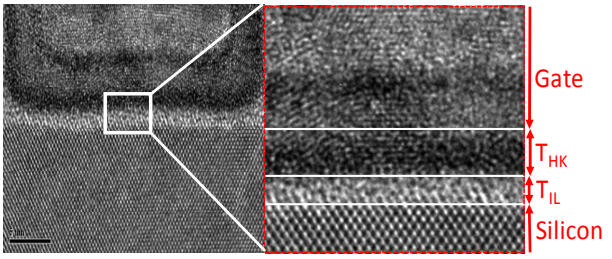

Fig. 1 Gate stack TEM images exhibiting HK and IL thicknesses of 1.45 and 1.27 nm, respectively.

To determine the gate stack parameters (offsets, thicknesses, dielectric constants, work function, doping concentration, etc.), we followed the previous work [7] by making a combination of the TEM image (see Fig. 1), the gate C-V fitting, and the conduction-band and valence-band electron tunnelling current fitting. Then substituting these parameters to our in-house microscopic MOS system simulator, we can transform the measured drain I-V at V_d = 0.05 V to the electron effective mobility as plotted in Fig. 2 versus inversion-layer density N_{inv}.

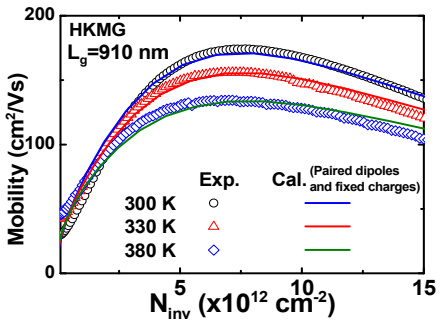

Fig. 2 Comparison of experimental (symbols) and simulated (lines) effective mobility at three temperatures. The simulation includes the fixed charges and "paired dipoles".

For the scattering by remote Coulomb charges (RCS), the experiment [3] shows that the flat-band voltage shift ΔV_{FB} changes slightly with HK layer thickness, This indicates that remote fixed charges are positive, with the density being around 3×10^{13} cm^{-2} at HK/IL as obtained from the ΔV_{FB} slope. On the other hand, the additional experiment [3], [5] and the *ab initio* results [8], [9] revealed that the dipoles are situated at the MG/HK interface and the HK/IL interface. In addition, the polarity of MG/HK dipoles is completely opposite to that at HK/IL as long as the metal gate contains the amount of silicon atoms [3].

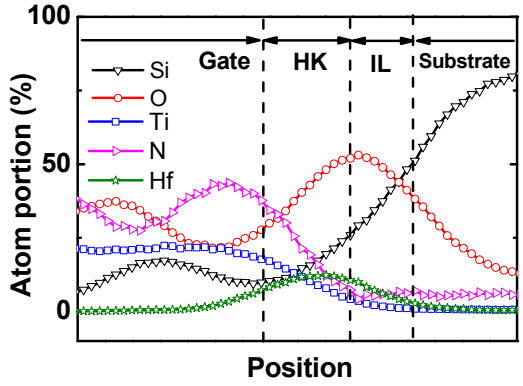

Fig. 3 Measured element distribution across the gate stack. Silicon atoms are quite rich in the metal gate, dictating that dipoles at MG/HK are opposite in polarity to those at HK/IL interface. This carries a negative threshold voltage shift to compensate for that from HK/IL dipoles.

Further, we present in Fig. 3 the element distribution measured across the gate stack. It can be seen that silicon is rich in the metal gate. As a result, the charge configuration involving fixed charges and dipoles is established in the present HKMG device sample, as depicted in Fig. 4.

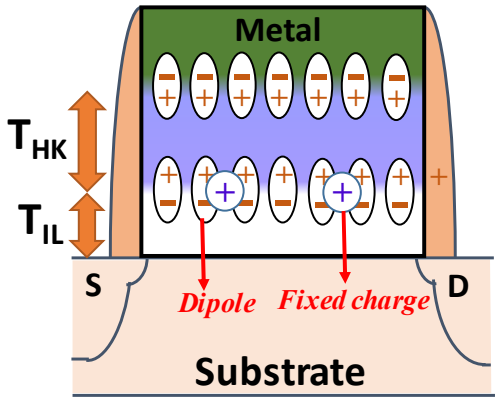

Fig. 4 Schematics of the dipoles at MG/HK and HK/IL interfaces as well as the fixed charges.

Formalism and Simulation

A. *Conventional Remote Dipole Scattering (RDS)*

In order to derive electron's momentum relaxation rate due to scattering by remote dipoles, it is necessary to solve a complicated three-dimensional Poisson equation with respect to one dipole configuration (shown in Fig. 5) at different boundaries. Stern [10] has greatly simplified the same problem by taking a cylindrical symmetry, with which the Poisson equation can be reduced to a one-dimensional differential equation (see appendix B of [10]).

The differential equation is given below:

$$\frac{\partial^2 A_k}{\partial z^2} - k^2 A_k - 2s\,\bar{A}_k\, g(z) = \frac{e}{2\pi\varepsilon}(\delta(z+z_0+\mathrm{d}) - \delta(z+z_0)) \cdots (1)$$

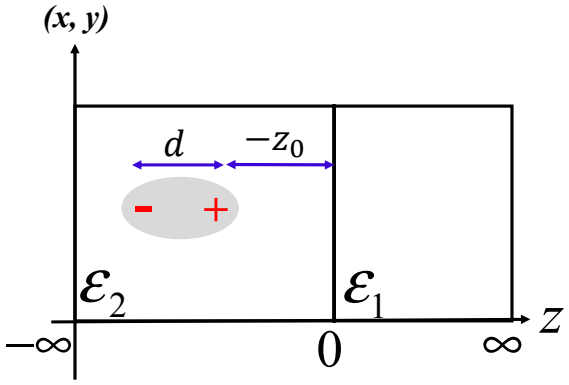

Fig. 5 Schematics of the charge configuration for the Poisson equation. The distance between the interface and the positive charge of the dipole is $-z_0$. The size of the dipole is d.

The corresponding charge configuration is shown Fig. 5. In Eq.(1), A_k is the remote one-dipole scattering amplitude associated with the potential (see [10]), and d is the dipole size. The physical meaning and values of remaining parameters can be found elsewhere [2]. One solution of Eq. (1) is:

$$\bar{A}(\mathrm{k}) = \int_0^\infty A_k(\mathrm{z})\,\mathrm{g}(\mathrm{z})\,\mathrm{dz} = \frac{e}{4\pi\varepsilon}\frac{P_0\,\mathrm{e}^{-kz_0}}{D}(1-\mathrm{e}^{-kd}) \cdots (2)$$

The solution $\bar{A}(\mathrm{k})$ can directly relate to that of RCS model [2] as long as the factor $(1\text{-}e^{-kd})$ reduces to 1.

The validity of (2) can be examined in the extreme limiting conditions, for instance, the term of $(1\text{-}e^{-kd})$ becomes 1 if the negative charge of the dipole leaves far from the positive charge ($d \to \infty$). In other case, the quantity $\bar{A}(\mathrm{k})$ of dipole becomes zero if those two charges within the dipole have complete overlap ($d \to 0$).

The solution of remote dipole scattering (RDS) rate incorporating the Born approximation [2], [11] can be written as

$$\frac{1}{\tau_{\mathrm{RDS}}} = \int_0^{2\pi} d\theta(1-\cos(\theta))\frac{2\pi m e^2}{\hbar^3} N_{dip}\,|\,\mathrm{A}(\mathrm{k},\mathrm{z}_0)\,|^2 \cdots (3)$$

Consequently, the total relaxation rate reads as

$$\frac{1}{\tau_{total}(E)}=\frac{1}{\tau_{SR}(E)}+\frac{1}{\tau_{Ph}(E)}+\frac{1}{\tau_{imp}(E)}+\frac{1}{\tau_{RCS}(E)}+\frac{1}{\tau_{RDS}(E)}\cdots(4)$$

In this work, the substrate dopant concentration is 4 x 10^{17} cm^{-3}, the effective permittivity is calculated by $\varepsilon_2 = 2\varepsilon_{ox}\varepsilon_{HK} / (\varepsilon_{ox}+\varepsilon_{HK})$ [6], and the size of the dipole d is equal to 4 nm (see [3] and [4]). Moreover, for RCS part, the fixed charge density at HK/IL is positive and has a value of 3×10^{13} cm^{-2} as determined from the experiment [3].

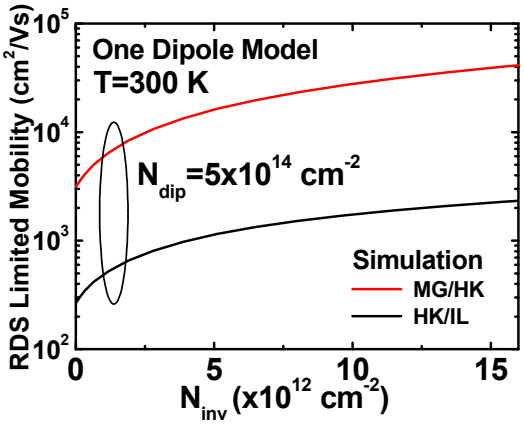

Fig. 6 Simulated RDS limited electron mobility versus inversion-layer density. The same interface dipole density is used in the simulation.

According to *ab initio* [4], the density of dipole at MG/HK is typical of up to 10^{14} cm^{-2}. Fig. 6 shows two RDS limited mobility curves thanks to dipoles at MG/HK and HK/IL interfaces, respectively. The mobility of MG/HK dipoles is two orders of magnitude larger than that of HK/IL dipoles, in case of the same dipole densities at each of two interfaces (5×10^{14} cm^{-2}).

Because of that, dipole density at MG/HK is assumed to be negligible in effect. We do not extract this quantity in this work, because these dipoles are not responsible for the mobility degradation. Consequently, the dipole density at HK/IL is the only parameter to be determined. To extract it, mobility simulation in this work is performed by considering the charge configuration as in Fig.4. This is involved with the self-consistent Schrödinger-Poisson equation solving to determine the underlying wave functions, followed by the Kubo-Greenwood formula for mobility calculation.

Fig. 7 shows simulation results in the "one dipole" model with and without fixed charges. The extracted dipole density at HK/IL is around 10^{15} cm^{-2} for fixed charges free case. This quantity yields a large ΔV_{th_dipole} of 12 V, which are comparable with that of Monte Carlo simulation [6]. Next, with the fixed charge density = 3×10^{13} cm^{-2} [3], the dipole density is reduced to 5×10^{14} cm^{-2}, along with a smaller ΔV_{th_dipole} of 5.5 V.

After considering RCS and RDS in the one-dipole model, the experimental effective mobility is well reproduced at 300 K. The fitting quality is good but the extracted dipole density and threshold voltage shift are still much higher than the published experimental and *ab initio* values.

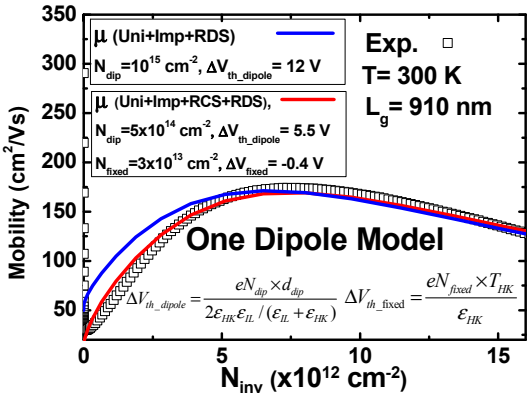

Fig. 7 Comparison of experimental (symbols) and simulated (lines) electron effective mobility versus inversion-layer density. One dipole model is used, with and without fixed charges, in the simulation.

B. "Paired" Remote Dipole Scattering (RDS)

Considering a circumstance where the dipole density is high enough, we can expect the potential of a dipole and its neighbor will have considerable "overlap", as shown in Fig. 8.

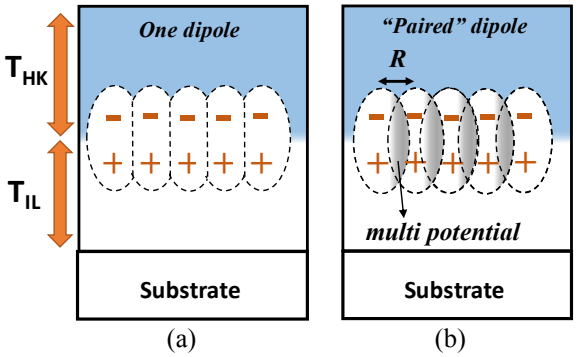

Fig. 8 (a) One dipole model by removing the overlap part of each dipole potential. As a result, the impact of dipoles is underestimated, leading to a large N_{dip} while fitting effective mobility data. (b) The "paired" dipole model including the overlap potential (shaded area), named as the multiple potential. The label R is the distance between a dipole and its neighbor.

These overlap areas of dipoles are remarkable. Those dipoles appear to be "paired" in terms of the created multiple potential as shown in Fig. 8 (b). Such multiple potential can strengthen the dipole's impact on mobility degradation. For the "paired" dipole model, we appropriately estimate the impact of multiple potential to a first-order approximation, by introducing a multiple potential factor [12] to multiply the amplitude associated

with potential A_k. In this case, A_k expression is therefore modified as

$$\overline{A}(\mathrm{k})_{paired} = \frac{e}{4\pi\varepsilon}\frac{P_0\,\mathrm{e}^{-kz_0}}{D}(1-\mathrm{e}^{-kd})(1+\frac{\sin(\mathrm{kR})}{kR}) \quad \cdots(5)$$

where R is the distance between paired dipoles and equals $\sqrt{4/\pi N_{dip}}$. Again, the mobility fitting quality is good as shown in Fig. 9. It is noteworthy that the extracted N_{dip} and ΔV_{th_dipole} are significantly reduced to 2×10^{14} cm^{-2} and 2 V, respectively, thanks to the application of the proposed "paired" dipole model.

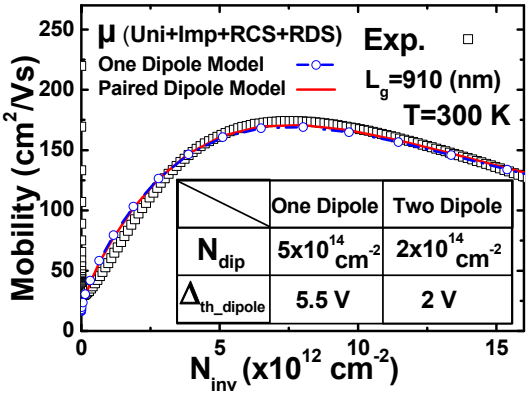

Fig. 9 Comparison of experimental (symbols) and simulated (lines) electron effective mobility versus inversion-layer density. Both dipole models are included in the simulation. The table lists the extracted N_{dip} and ΔV_{th_dipole} values.

Results and Discussion

Using the same input parameters, the temperature dependent inversion-layer electron effective mobility has been well reproduced within the context of the paired dipole model, as shown in Fig. 2, achieved without adjusting any parameters.

More importantly, the extracted dipole density in this work is much smaller than that of Monte Carlo simulation [6], leading to a threshold shift as small as 2 V. The underlying dipole density at HK/IL is around 2×10^{14} cm^{-2}, which is quite close to both the experimental observation [3] and the *ab initio* calculation [4].

There are several factors to affect the total threshold voltage shift ΔV_{th}. First, the experimentally determined fixed charges at HK/IL interface is around 3×10^{13} cm^{-2} [3]. These fixed charges carry a threshold voltage shift of -0.4 V. Second, MG/HK dipoles are opposite in polarity to those at the HK/IL interface. The corresponding dipole density is *nearly* equal in magnitude to each other (around 10^{14} cm^{-2}). Consequently, the net threshold voltage shift is likely small in magnitude, taking into account fixed charges and dipoles, thanks to charge compensations.

Conclusion

Through the microscopic mobility calculation and the experimental comparison, the proposed "paired dipoles" configuration has been verified to be a plausible intrinsic origin of the mobility reduction in HKMG MOSFETs.

Acknowledgment

This work was supported by the Ministry of Science and Technology of Taiwan (Grant no. 104-2221-E-009-072-MY3 and 104-2221-E-009-058-MY3).

REFERENCES

[1] M. Cassé, et al., "Carrier transport in HfO_2/metal gate MOSFETs : Physical insight into critical parameters," *IEEE Trans. Electron Devices,* vol. 53, no. 4, pp. 759–768, 2006.

[2] N. Yang, et al., "Estimation of the effects of remote charge scattering on electron mobility of n-MOSFET's with ultrathin gate oxides," *IEEE Trans. Electron Devices*, vol. 47, no. 2, pp. 440–447, 2000.

[3] M. Kadoshima, et al., "Two different mechanisms for determining effective work function ($\Phi_{m,eff}$) on high-k- Physical understanding and wider tunability of $\Phi_{m,eff}$," in *Proc. IEEE Symp. VLSI Technol.,* 2006, pp. 180–181.

[4] O. Sharia, et al., "Theoretical study of the insulator/insulator interface: Band alignment at the SiO_2/HfO_2 junction," *Phys. Rev. B*, vol. 75, no. 3, p. 035306, 2007.

[5] H. Ota, et al., "Intrinsic origin of electron mobility reduction in high-κ MOSFETs—From remote phonon to bottom interface dipole scattering," in *Proc. IEEE IEDM.*, 2007, pp. 65–68.

[6] P. Toniutti, et al., "On the origin of the mobility reduction in n- and p-metal-oxide-semiconductor field effect transistors with hafnium-based/metal gate stacks," *J. Appl. Phys.*, vol. 112, no. 3, p. 034502, 2012.

[7] M. J. Chen, et al., "Temperature-oriented mobility measurement and simulation to assess surface roughness in ultrathin-gate-oxide (~1 nm) nMOSFETs and its TEM evidence," *IEEE Trans. Electron Devices*, vol. 59, no. 4, pp. 949–955, 2012.

[8] A. G. Van Der Geest, P. Blaise, and N. Richard, "*Ab Initio* study of the electrostatic dipole modulation due to cation substitution in HfO_2/SiO_2 interfaces," *Phy. Rev. B.,* vol. 86, pp. 085320, Aug. 2012.

[9] C. L. Hinkle, et al., "Dipole controlled metal gate with hybrid low resistivity cladding for gate-last CMOS with Low Vt," in *Proc. IEEE Symp. VLSI Technol.,* 2010, pp. 183-184.

[10] F. Stern, "Polarizability of a two-dimensional electron gas," *Phys. Rev. Lett.*, vol. 18, no. 14, pp. 546–548, 1967.

[11] K. Hess, "Impurity and phonon scattering in layered structures," *Appl. Phy. Lett.,* vol. 35, pp. 484, Oct. 1979.

[12] H.Kosina and G. Kaiblinger-Grujin, "Ionized-impurity scattering of majority electrons in silicon," *Solid-State Electron.*, vol. 42, pp. 331–338, 1998.