P2-14
Importance of Exact Modeling for Gate poly-Si of MOSFETs with Ultra-thin Oxide

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1. Introduction
Marvelous amounts of development costs make semiconductor business to be risk full, which strongly requires a highly precise device simulation. Since today's device simulations, however, assume the Boltzmann approximation (BA) that is a bad approximation in a high concentration layer of semiconductor devices integrates in LSI; there inherently exist theoretical errors from the Fermi-Dirac statistics due to the BA. The errors must accordingly hide in the conventional device simulations, if a gate insulator thickness becomes so thin for us to take into account a heavily doped gate poly-Si. With a given electron density, the BA lowers the Fermi level (E_F < E_p), as schemed in Fig. 1, in a degenerate semiconductor. It is noteworthy to say that we should carefully consider such an inherent error due to the BA besides direct tunneling through the gate insulator when we simulate ultra-thin gate oxide MOSFETs that cannot suppress gate leakage current. Our goal of this article is to reveal the error due to the BA by using a self-consistent calculation of the threshold voltage (V_TH).

2. Present approach
In order to investigate the inherent error due to the BA, we have developed one-dimensional specified simulator (DT1d) including two options: (1) The BA is assumed. (2) The Fermi-Dirac statistics is assumed. Of course, the option (2) is exact. DT1d calculates CV and JV curves of MOS capacitor, taking into account the following phenomena: (a) impurity ionization rates, (b) band-gap narrowing (BGN), (c) poly-Si depletion, (d) interface quantization, and (e) the direct tunneling through the gate oxide. The phenomena (a) and (b) play a central role of the present approach because these two operate mutually to define the Fermi level of electron-hole system in semiconductor [1]. Fig. 2 shows that the BA results in the complete ionization in the range of N_D where BGN is overestimated. Therefore, the BA isn't appropriate in the range of N_D > 1e19 (cm^-2). The phenomenon (e) is involved because DT1d solves the Poisson equation including gate poly-Si. The phenomena (d) comprises of four components: (d1) electron quantization at the substrate surface, (d2) hole quantization at the substrate surface, (d3) electron quantization at the poly-Si surface, and (d4) hole quantization at the poly-Si surface. DT1d involves these four all in the Poisson equation. The interface quantization, as a result, refines accumulations of carriers in the gate poly-Si, since the accumulation layer width is too small to confine neither electrons nor holes in the poly-Si surface. The phenomenon (e) is included while solving the Poisson equation. These all phenomena relate each other as follows: (a), (b), and (d). The interface quantization modulates carrier densities, so the Fermi level shifts. Then, the ionization rate and BGN modulate and affect on the solution of the Poisson equation. In such a way, the phenomena (a)-(e) have a deep and complex relation. DT1d self-consistently calculates CV and JV curves by including these all phenomena in the same Poisson equation.

3. Results
Fig. 3 shows that the BA underestimates the gate current in the substrate depletion regime (V=−1 (V) to 0(V)), since the poly-Si concentration (N_poly) is so high (1e20 (cm^-3)) that the BA underestimates the absolute of the flat band potential (V_TH), as shown in Fig. 4. The gate current is in proportion to |V_TH| in the substrate depletion regime. Fig. 5 shows that the capacitance is rather large near V=−2 (V), so overestimates the oxide thickness (t_ox), as will be described below. Fig. 4 further shows that the BA overestimates the V_TH. The relativistic errors in V_TH and V_FB shown in Fig. 6 are more than 25(%) and more than 10(%) when N_poly>1e20 (cm^-3), respectively. These errors are 20 times larger than those when assuming the complete ionization. Fig. 7 summarizes the temperature and N_poly dependencies of the error due to the BA in V_TH in which the error increases with N_poly and decreases with the temperature. The temperature dependence is the evidence that the BA approaches to be exact when temperature becomes so high. It should be noted that the error in V_TH is very high, i.e., nearly 90 (mV) at 300 (K) and still 80 (mV) at 400 (K). This strongly suggests that we should develop the foundation of the device simulation grounded on the Fermi-Dirac statistics in near future. Fig. 8 shows that the error due to the BA in t_ox increases with N_poly and decreases with the temperature.

4. Conclusion
If we didn't perform the above self-consistent calculation between the ionization rate and BGN, then we couldn't find the inherent errors due to the BA. Neglecting the self-consistent calculation, for example, results in that the error in V_TH is less than 5 (mV) which means about 1 (%) when N_poly=1e20 (cm^-3) at 300 (K). It is because the BA, as is clearly shown in Fig. 2, obtains the same result as is obtained by assuming the complete ionization [1]. Therefore, both the Fermi-Dirac statistics and the self-consistent calculation are necessary to perform an appropriate device simulation. The present approach obtains the first evidence indicating that the error due to the BA in V_TH is greater than 70 (mV) and that the error due to the BA in t_ox is greater than 3 (Å).

Acknowledgements
This work has been supported by Mr. H. Tanimoto, Toshiba Semiconductor Company and has been encouraged and helpfully advised by Mr. K. Matsuzawa.

References
Fig. 1 Error due to the Boltzmann approximation in electron density.

Fig. 2 Errors due to the Boltzmann approximation in BGN and the ionization rate while at 300(K).

Fig. 3 Error due to the Boltzmann approximation in JV curve while N_D=2.5e16 (cm^-3), N_poly=1e20 (cm^-3), and t_OX=1.98(nm) at 300(K).

Fig. 4 The poly-Si concentration dependence of the errors due to the Boltzmann approximation in V_TH while N_D=1e15 (cm^-3), and t_OX=1.98 (nm) at 300 (K).

Fig. 5 Error due to the Boltzmann approximation in CV curve while N_D=2.5e16 (cm^-3), N_poly=1e20 (cm^-3), and t_OX=1.98 (nm) at 300 (K).

Fig. 6 The poly-Si concentration dependence of the relativistic errors due to the Boltzmann approximation in V_TH while N_D=1e15 (cm^-3), and t_OX=1.98 (nm) at 300 (K).

Fig. 7 Temperature and N_poly dependencies of the errors due to the Boltzmann approximation in V_TH while N_D=1e15 (cm^-3), and t_OX=1.98 (nm). The temperature dependence is shown while N_poly=3e20 (cm^-3) and the N_poly dependence is shown while the temperature is 300 (K).

Fig. 8 Temperature and N_poly dependencies of the error in the oxide thickness while t_OX=2 (nm), and N_D=2.5e16 (cm^-3). Temperature dependence is shown while N_poly=1e20 (cm^-3) and the N_poly dependence is shown while the temperature is 300 (K).