Correlation between the Material Properties of the High-K Gate Dielectrics

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Currently, an active area of research in microelectronics, is dielectrics, with a high dielectric constant, κ, as a possible replacement for SiO2, as the gate dielectric, in future MISFETs.1 The high-κ dielectrics have been reviewed recently.2-4 For carrying out a comparative evaluation of the merits and the demerits of the high-κ materials in a systematic manner, it is necessary, first, to identify the critical issues, on which a gate dielectric is to be assessed, and then analyze their inter-linkages, so that the profile of an optimal high-κ gate dielectric can be outlined, against which the different high-κ dielectrics can be compared and ranked. These were the aims of this work.

In many respects, the dry thermal SiO2 is as perfect a gate dielectric as any one can get.2 Interestingly, its near perfection in some respects can be said to have been its unmaking, when its application in sub-70-nm MISFETs is concerned. The basic factors, that promote its huge band gap (nearly 9.0 eV), which provides large energy barriers (nearly 3.2 and 4.7 eV, respectively) to both electron and hole transport, and its higher covalency and fourfold coordination, which contribute to very low interface/bulk defect density, inevitably lead to one of the lowest dielectric constants among all inorganic insulators and also one of the lowest specific densities. In a high quality solid with structural symmetry and low defect density, the combination of high band gap (desirable for low MISFET off current) and covalent bond (desirable for high quality interface with resultant higher carrier mobility and device reliability), with high dielectric constant (to satisfy the perrenial need for higher drain current) and high specific density (desirable for low diffusion constant), is likely to be rare. One could obtain a high dielectric constant in a high band gap solid by increasing ionicity (ionic polarization), structural asymmetry (dipolar polarization), and/or defect density (defect and/or space charge polarization), however, these may generate reliability problems and frequency-dependent dielectric constant with multiple relaxation frequencies (f), some of which will be lower than the clock frequency (>> 1 GHz).

Most of the important material constants of the high-κ dielectrics are interlinked. Perhaps, the most basic element that links these properties is the nearest neighborhood, which may be assessed, and then analyze their inter-linkages, so that the profile of an optimal high-κ gate dielectric can be outlined, against which the different high-κ dielectrics can be compared and ranked.

The coordination number (CN) may be an important parameter determining the stability of the high-κ dielectrics as well the quality of the Si/ high-κ-dielectric interfaces. For this objective, the most desirable CN may be 4 (which both Si and SiO2 have, facilitating the highest quality interface, technology has ever achieved), which, unfortunately, none of the high-κ dielectrics has, because of higher ionicity. For some high-κ gate dielectrics, high CN appears to lead to structural asymmetry and inter-conversion between alternate nearest neighbor configurations. The uncommon CN of 7, which occurs for a number of the high-κ dielectrics (such as ZrO2, HfO2, La2O3) appears to have uncommon features, including unequal cation-anion distances, (in ZrO2, HfO2, all seven M-O distances are reported to be different, while in La2O3, 3 different sets of distances may exist). It has been suggested, that in the case of sevenfold coordination, stoichiometry and charge balance are maintained with half the anions having a coordination of 3 and the rest of the anions having a coordination of 4. Whether the center of gravity of the cations is the same as that of the anions in these dielectrics (when the CN. = 7) is an important question. If not, there may be a contribution to κ from dipolar polarization.

The contribution of the electronic polarization to the dielectric constant, $\kappa_{\text{electric}}$, (f = 10^{15}-10^{16} Hz), should be about n$^2$ (where n is the refractive index),2-4 which even in the case of low bandgap (e.g. TiO2) or heavy cations (e.g. HfO2) does not exceed 7. (In Si and diamond, $\kappa_{\text{electric}}$ = n$^2$, which confirms that there is no polarization in these solids other than electronic. The Moss Rule suggests an inverse relation between $\kappa_{\text{electric}}$ and Eg.5) The remaining dielectric constant, $\kappa_{\text{static}}$ = $\kappa_{\text{electric}}$, is contribution from ionic, $\kappa_{\text{ionic}}$ (f = 10^{10}-10^{13} Hz), dipolar (f = 10^{10}-10^{13} Hz), defect (f = 10^{-10}{10^{12}} Hz), and space-charge (f = 10^{-10}{10^{12}} Hz) polarizations.

In dry thermal SiO2 and in Al2O3, the dielectric constant has been found to be independent of frequency from low to very high frequencies. Therefore, it can be assumed that in dry thermal SiO2 and in Al2O3, there is only electronic and ionic polarizations with $\kappa_{\text{electric}}$ = 6 and 6.6, respectively. As already pointed out, only $\kappa_{\text{electric}}$, Bond type will be useful for the gate dielectric capacitance at the clock frequency, while the other polarizations will only create reliability problems.

Based on our identification of the critical material constants and our analysis of their inter-linkages, we have outlined an approximate profile of the optical high-K gate dielectric with clock-frequency $\kappa$ = 18, Eo = 6.0 eV, $m^*$ = 1.0 m, $\chi = 1.6$ eV, $\rho$ = 5.0 g/cm$^3$, $\alpha = 2.5X10^{-4}$, and CN. = 4.0. Compared to this (hypothetical) benchmark gate dielectric, Al2O3 has the highest rank, followed by Al2O3, ZrSiO2, ZrO2, La2O3, and Y2O3, while BaZrO2, Ta2O5 and TiO2 compare poorly. From our analysis, it appears unlikely that any high-κ binary dielectric will attain the optimal values of all the important bulk parameters. (The score for HfO2 is 7.46 against 10 for the optimal gate dielectric.) High-κ silicates or oxide solid solutions have to be found that effectively combine the attractive properties of the high band gap oxides (e.g. $E_0$, $\chi$, and CN. of SiO2) with those of the high-κ oxides (e.g. $\kappa$, $\rho$ of HfO2 and Ta2O5).