512e Design Organic Self-Assembly Monolayers (Sams) on Silicon Surface as Low K and High K Dielectric Materials Applied in Nanoelectronics

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With continuing device scaling beyond the 90nm node, the dielectric materials become extremely important in limiting chip density and performance. For example, the wiring interconnect requires a low k dielectric replacing silicon dioxide to reduce the signal delay, cross-talk and power dissipation. At other hand, the gate in field effect transistor (FET) requires a high k material replacing silicon dioxide to improve signal responding, dielectric breakdown voltage even at several adatom layers. Those nano-scale dielectric materials are one of key problems to enabling the semiconductor industry to achieve the ultimate CMOS device. Here we report the computational design of the novel organic self-assembly monolayers on silicon surface functioning as targeted dielectric materials. We have been developing a multi-scale hierarchy simulation method to predict the dielectric properties of bulk crystals, self-assembly thin films and device structures. This hierarchy simulation method bridging the atom precise to entire device involves the first principle calculation, the molecular dynamics with polarizable force field, the finite element method (FEM) modeling. Thus we use first principle methods to calculate the bulk dielectric properties, simulate the dielectric properties of organic SAM with first-principle derived polarizable force field and model the nanoelectronic devices with parameters achieved by simulation. By this manner, we avoid any empirical misleading and thus can predict accurately the proposed nano-structured dielectric materials. With alterative simulation/experiment efforts, we have demonstrated several low k or high k organic SAMs for nanoelectronics.