# Comparison of Voronoi and Cuboid Methods for Work Function Fluctuation and Suppression by Using Stacked-metal Gate on Gate-All-Around Nanowire n-MOSFETs

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## Abstract

We for the first time compare  $V_{th}$  variability ( $\sigma V_{th}$ ) induced by work-function fluctuation (WKF) using the Voronoi and cuboid methods on silicon (Si) gate-all-around (GAA) nanowire (NW) n-MOSFETs. We do propose a TiN/TaN stacked gate to suppress WKF-induced  $\sigma V_{th}$ . Our main findings indicate the magnitude of  $\sigma V_{th}$  is comparable between the Voronoi and cuboid methods. Moreover, the Voronoi grain pattern shows abrupt electric field between the grains of low and high work-function (WK), and interface between channel and source/drain extensions due to more grains with low WK surrounding the grain with high WK. A stacked TiN/TaN metal-gate is further examined, which can effectively reduce  $\sigma V_{\text{th}}$  up to 43.5%.

### 1. Introduction

GAA NW MOSFETs with high-k/metal-gate technology owns excellent electrical characteristics to replace FinFETs in emerging technology [1-2]. However, WKF is a major variability due to grain orientations in small metal gate area [3]. Many papers have studied the effect of nano-size grain metal by using different methods, such as averaged WKF method [4], cuboid method [5], and Voronoi method [6-7]. Currently, only the cuboid method can approximate real grains to quantize the metal grain number (MGN) at the same grain size for the effect of the metal grain number and metal grain location. Moreover, the cuboid method can apply to predict the variability by physical models of grain number with different probabilities (p) and values of WK. However, a unified comparison between these two methods has not been investigated clearly for GAA NW devices.

In this work, we propose a newly developed technique of Voronoi method to estimate the  $\sigma V_{th}$  induced by the WKF with three MGNs (16, 80, and 320). We do compare it with the result of the cuboid method. Physical analysis is investigated; and, we propose a TiN/TaN stacked gate to suppress the  $\sigma V_{th}$  by the cuboid method [8].

# 2. Simulation Methodology

An experimentally validated three-dimensional (3D) quantum-mechanically-corrected transport model was employed [9]. Fig. 1(a) shows the studied device with nanosized TiN metal grains, where the simulated structure comprises a metal gate TiN/high-κ HfO<sub>2</sub> stack with a cylindrical Si channel. Fig. 1(b) outlines the flow of Voronoi method. First, we set the grain size and dimension of metal gate in our program to generate Voronoi diagram, as shown in Fig. 1(c). Second, we transform the Voronoi diagram to 3D coordinate for device simulator to create the Voronoi grain patterns for different average grain sizes (4x5, 2x2, 1x1 nm<sup>2</sup>). Then, according to TiN's grain orientations [10–11], we set TiN<111> (p = 0.4, WK = 4.43 eV), TiN<200> (p = 0.6, WK = 4.63 eV), and 300 simulated cases in Monte Carlo (MC) program. Finally, we randomly generated 300 statistically random Voronoi grain patterns with random WKs, as shown in Fig. 1(d). For a fair comparison with cuboid method [5], we generated the same grain numbers with various grain sizes for both the Voronoi and cuboid methods.

## 3. Results and Discussion

Figure 2 presents the cumulative probability of V<sub>th</sub> induced by the WKF with respect to three total grain numbers for Voronoi and cuboid method, where Vth is extracted by a constant current  $(3.14 \times 10^{-8} \,\mu\text{A})$  from the I<sub>D</sub>–V<sub>G</sub> curve. We observed that the distributions of V<sub>th</sub> for both the Voronoi and cuboid method were close to continuous Gaussian distributions without outlier points. However, it differs from previous study using the cuboid method or square method [7]. Fig. 3 shows the comparison of conduction band energy distribution, and electric field for the Voronoi and cuboid method in the on-state  $(V_G = V_D = 0.6 \text{ V})$  at the channel surface along the channel position from source (S) to drain (D). Clearly, the conduction band energy distribution was affected seriously for Voronoi grain pattern with more grains of low WK surrounding the grain with high WK, as shown in Fig. 3(a). Then, the Voronoi grain pattern shows abrupt electric field near boundary from the grain with high WK to low WK, and interface between channel and S/D extensions, as shown in Fig. 3(b). For a fair comparison to other researcher's study between different average grain size (GS) and area of metal gate (AG), Fig. 4 shows the comparison of the  $\sigma V_{th}$  with various GS/AG [6] for the Voronoi and cuboid method. It is observed that magnitude of  $\sigma V_{th}$  is comparable for both Voronoi and cuboid method. It implies that cuboid method can be used to approximate the real grains very well. Fig. 5 shows the  $\sigma V_{th}$  induced by the WKF with TiN and stacked TiN/TaN metal gate. We found that stacked TiN/TaN metal gate can reduce 43.5% of the magnitude of  $\sigma V_{th}$  as compared to TiN metal gate due to more random MGNs.

#### 3. Conclusions

In summary, the cuboid method can be applied to approximate the real grains very well for WKF as compared to the Voronoi method. The cuboid method is the best way to quantize the grain number and analyze the physical models for WKF. Based on the cuboid method, the magnitude of  $\sigma V_{th}$ can be suppressed effectively by TiN/TaN stacked metal-gate.

#### Acknowledgment

This work was supported in part by the Ministry of Science and Technology, Taiwan, under Grant MOST 106-2221-E-009-149, Grant MOST 106-2622-8-009-013-TM, Grant MOST 107-2622-8-009-011-TM, Grant MOST 107-2221-E-009-094, and Grant MOST 107-3017-F-009-001, and in part by the "Center for mmWave Smart Radar Systems and Technologies" under the Featured Areas Research Center Program within the framework of the Higher Education Sprout Project by the Ministry of Education, Taiwan.

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Fig. 1. (a) Schematic of the GAA NW device with metal grains, where the gate length is 10 nm, the radius of cylindrical channel is 5 nm, and the effective oxide thickness is 0.6 nm. (b) Flow chart of Voronoi method. (c) Voronoi diagram. (d) Random WK with different grain orientations.



Fig. 3 Comparison of (a) Conduction band energy distribution, and (b) Electric field for the Voronoi and cuboid method in the on-state ( $V_G = 0.6 \text{ V}$ ,  $V_D = 0.6 \text{ V}$ ) at the channel surface along the channel position from S to D.



Fig. 4. Comparison of the  $\sigma V_{th}$  with various GS/AG for the Voronoi and cuboid method.



Fig. 5. The  $\sigma V_{th}$  induced by the WKF with TiN and stacked TiN/TaN metal gate, where the grain size is 2x2 nm<sup>2</sup>.