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Comparative study in work-function variation: Gaussian vs. Rayleigh distribution for grain size

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Abstract: Because of the significantly-increasing work-function variation (WFV) in high-k/metal-gate technology in sub-30-nm nodes, a simple but reasonable model for quantitatively estimating the WFV is currently required. In this study, a Monte Carlo simulation for statistically generating the grain sizes following two different probability distributions (*i.e.*, Gaussian and Rayleigh distributions) is suggested and performed. The shapes of the grains created by following the Rayleigh distribution (*vs.* the Gaussian distribution) are significantly closer to the real shapes of the grains in the metal gate of TiN. Thus, the WFV estimated by using the Rayleigh distribution is well matched to the previous results.

Keywords: work-function variation, variability, Monte Carlo simulation
Classification: Electron devices, circuits, and systems

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1 Introduction

In state-of-the-art nanometer-scale metal-oxide-semiconductor field-effect transistors (MOSFETs), the effects of both the systematic (*e.g.*, variation in effective/physical channel length and width, gate oxide thickness, and source/drain junction depth) and random variations (*e.g.*, line edge roughness (LER), line width roughness (LWR), random dopant fluctuation (RDF), and work-function variation (WFV)) on device parameters are significant, which pose challenges for the continuous scaling of MOS devices, especially in sub-30-nm technology nodes. In order to address these technical issues (*i.e.*, to reduce systematic/random variation), advanced transistor architectures such as ultra-thin-body devices and multi-gate devices have been widely studied and several are currently being adopted in production.

Several studies for estimating random parametric failures caused by LER/LWR and RDF have been performed. A few studies on WFV modeling, however, have been performed [1, 2], and an experimental study on WFV has been demonstrated [3]. In this study, a Monte Carlo (MC) simulation is used to generate arbitrary grain sizes by following two different probability distributions (*i.e.*, Gaussian and Rayleigh distributions) in a given limited gate area of a high-k/metal-gate (HK/MG) device in order to improve the physical validity of the model (section 2). To build the validated model, the generation of grain shape is primarily considered in this study. Based on the MC simulation results and the use of the ratio of the average grain size to the gate area (RGG), a simple way of quickly estimating the WFV for a given metal material is suggested that is independent of the grain size (section 3). Lastly, it is concluded that the WFV estimated by using the Rayleigh distribution (*vs.* the Gaussian distribution) is well matched to the previous experimental and three-dimensional simulation results.

2 Monte Carlo simulations for WFV, using Rayleigh and Gaussian distributions

Fig. 1(a) shows the flow chart of the procedure used to estimate the work-function (WF) in a device. For a given gate area and average grain size (*e.g.*, TiN with an average grain size of 4.3 nm [3] in a gate area of 30 nm × 40 nm), the grains are randomly generated under the condition that their sizes follow a Gaussian or Rayleigh distribution. Fig. 1(b) and 1(c) shows an example of TiN metal grains following the Gaussian and Rayleigh distributions, respectively. Then, the orientation of each grain that is generated is statistically assigned by referring to the table of characteristics [4]. Lastly, the WF is calculated for each device (total of 10^5 devices) by using the equation in the fourth box in Fig. 1(a), where x_i (i = 1 to N) is the probability value of the assigned grain orientation, N is the total number of grains in each device, and Φ_{xi} is the WF value of the assigned grain orientation. The overall shape of the grains in Fig. 1(b) is similar to what was shown in [2] where the grains in a metal gate are partitioned into several square-shaped sub-regions in order to simply estimate the WFV. In fact, the overall shape of the grains shown in Fig. 1(c) is more realistic because several smaller grains combine with each other and become a larger

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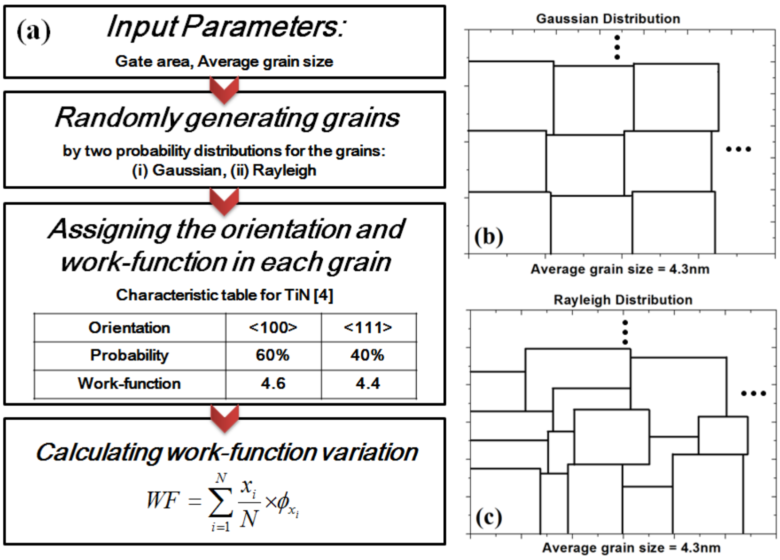

Fig. 1. (a) Flow chart for calculating the WF for a device. An example of metal grains (where the average grain size of carbon-incorporated TiN is 4.3 nm [3]) following a (b) Gaussian distribution and (c) Rayleigh distribution.

grain, instead of splitting into smaller grain sizes. Similar grain shapes are also simulated and utilized in [1], where a large real granular image is used to sample a gate area for a MC simulation. As a result, the number of grains (total of 10^5 samples) in Fig. 1(b) exists in a relatively narrower range than in Fig. 1(c), as shown in Fig. 2(a).

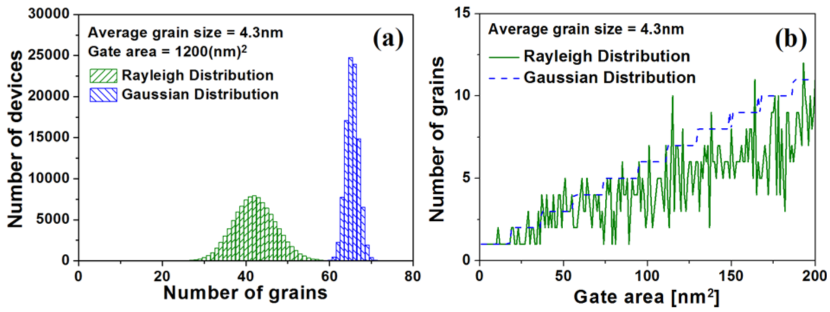

Fig. 2. (a) Number of devices (total of 10^5 samples) *vs.* the number of grains. Note that all the transistors (W/L = 40/30 nm) do not have an identical number of grains. (b) Number of grains *vs.* gate area.

Depending on the distribution that the grain sizes follow, the number of grains increases with the gate area, as shown in Fig. 2(b). In the case of the Rayleigh distribution, the number of the grains stochastically increases with increasing gate area. In the case of the Gaussian distribution, interestingly, a step-like shape is obtained. This originated from the fact that because the average grain size is significantly smaller than the gate area, the number of grains is almost constant when the gate area is increased by only a small amount.

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3 Results and discussion

According to the previous studies [1, 2], an amorphous metal gate is preferred to suppress the WFV in devices; therefore, it can be deduced that a critical gate area meeting the variation targets (or statistical corners) would exist, once a gate material is chosen. Based on the deduction, we take advantage of the RGG (*i.e.*, ratio of average grain size to gate area) [5] in this study (Fig. 3).

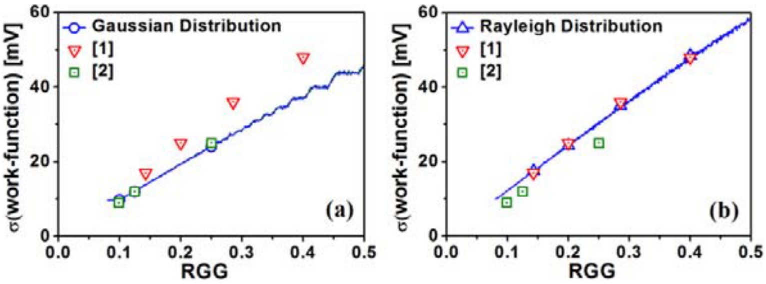

Fig. 3. σ(WF) *vs.* RGG for two different distributions: (a) Gaussian and (b) Rayleigh. Note that the more realistic 3-D simulation results [1] and the simple analytical model that is only using square-shaped grains [2] are indicated in the plots together in order to show the validity of the RGG by comparing it with previous results [1, 2].

As a result of using the Gaussian distribution for creating the grains, the total number of grains is almost constant over a minuscule increase in RGG (shown in Fig. 3(a)), so the curve shape in the plot of σ(WF) *vs.* RGG resembles a step (the reason has already been described in the section 2). In addition, as the gate area is scaled down (*i.e.*, RGG is increased) without any decrease in the average grain size, the Gaussian distribution used to generate the grains does not correctly estimate the WFV (Fig. 3(a)). As shown in Fig. 3(b), however, σ(WF) obtained from the grain sizes following the Rayleigh distribution is consistent with the previous results [1, 2] because several smaller grains in metal gate stacks can be easily combined with each other in annealing processes or any type of heat-treatment processes for the HK/MG. This results in a larger grain size, rather than

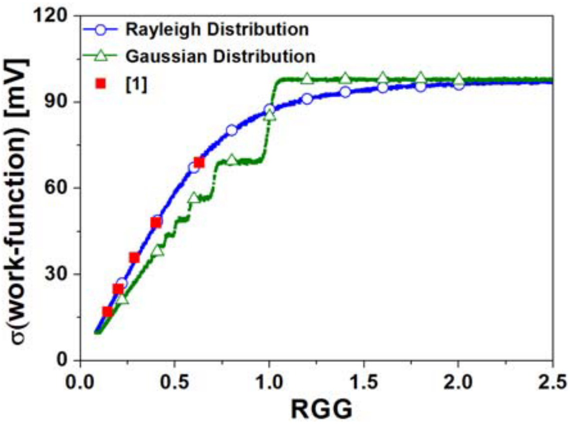

Fig. 4. σ(WF) *vs.* RGG. Note that the average grain size of the C-incorporated TiN is 4.3 nm.

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splitting into smaller grain sizes. Hence, the Rayleigh distribution (*vs.* the Gaussian distribution), which has a longer tail on one side, is more realistic and physically valid for generating various grain sizes.

Fig. 4 is plotted in the range of RGG < 2.5. The WFV obtained by using the Gaussian distribution is underestimated in the range of RGG < 1.0, mainly because the number of grains in all sample devices is greater if the Gaussian distribution is used for generating the grains (also shown in Fig. 2(a)). However, regardless of the type of distribution that is utilized for creating the grain sizes, the upper limit of the WFV can still be reasonably estimated, in the scenario that the grain size is no longer scaled down, but the gate-area is continuously scaled down (*i.e.*, RGG >1).

4 Conclusion

In this study, a Monte Carlo (MC) simulation has been employed to generate arbitrary grain sizes following two different probability distributions (*i.e.*, Gaussian or Rayleigh distribution). The shapes of the grains created by following the Rayleigh distribution (*vs.* the Gaussian distribution) are significantly closer to the real shape of the grains in the metal gate of carbon-incorporated TiN because several smaller grains combine with each other and become a larger grain, instead of splitting into smaller grain sizes. As a result, the work-function variation (WFV) is underestimated by using grains created with the Gaussian distribution, but the WFV with the grains following the Rayleigh distribution is well matched to the previous results. Therefore, when the grain sizes in metal gates are generated to estimate the WFV, the Rayleigh distribution is more realistic than the Gaussian distribution.

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