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Modeling and physical mechanism analysis of the effect of a polycrystalline-ferroelectric gate on FE-FinFETs

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Due to its potential in low-power computing or storage applications, the HfO_2-based ferroelectric (FE) field-effect transistor (FET), which consists of a MOSFET and an FE gate dielectric stack on the top of the original gate, has attracted massive research interest in the past decade [1]. Taking advantage of the scalability of FE HfO_2-based film [2], FE-FETs have been developing high-performance computing and high-density memory at advanced process nodes [3]. However, significant variations in state-of-the-art FE-FinFETs are also caused by polycrystalline FE gates. The HfO_2-based FE film microstructure is microscopically disordered and polycrystalline, with the grain varying spatially in terms of radius, phase distribution (FE orthorhombic, non-FE monoclinic, and tetragonal phases), and orientation [4]. As the dimension scales down, the FE gate of an FE-FET may contain a few randomly distributed grains and can no longer be considered a monocrystal film. The random distribution of grains induces a new source of variability into the FE-FinFETs, which is comparable with those induced by other traditional sources [5].

The physical mechanism of FE-FinFET variability induced by polycrystalline FE gate is investigated in detail in this study. To describe the polycrystalline FE HfO_2-based film, a multi-grain (MG) FE model is proposed, which includes irregular grain shape, different phases (FE and non-FE phases), and different grain orientations. To create an MG FE-FinFET model, the MG FE model was introduced to a 7 nm bulk FinFET TCAD platform. The MG FE-induced statistical variability of the key figures of merit (FoM) for FE-FinFETs is described using the MG FE-FinFET model. Finally, by analyzing FE polarization and channel electrostatic potential, the physical mechanism of FE-FinFETs performance variation associated with polycrystalline FE is studied and discussed.

Multi-grain ferroelectric model. Referring to the microstructure of HfO_2-based FE film observed in experiments [4], an MG FE film model is established, considering irregular grain shapes, different grain phases, and grain orientations, illustrated in Figure 1(a). The irregular grains are generated by the Voronoi tessellation algorithm [6], and the FE and dielectric (DE) grains are determined by the grain size [7]; moreover, the distribution of grain orientations is described by the Gaussian distribution, a common model to be used in the simulation. The effect of grain orientation is shown in Figure 1(b). With an angle θ between polarization (P) and electric field (E), the intrinsic P-E characteristics have to be rewritten following the parallelogram law. In addition, a 7-nm n-type FE-FinFET TCAD model has been developed based on the FinFET platform and the Landau-Khalatnikov (L-K) model. The detailed modeling process and parameters of the baseline-FinFET and FE layer are described in Appendix A.

MG FE-induced statistical variability of FE-FinFET. In the following, to investigate the effect of a polycrystalline FE gate, the MG FE microstructure patterns and modified L-K model are introduced into the FE-FinFET. Figure 1(c) displays 100 simulation results of transfer characteristic curves of MG FE-FinFETs with distinct FE layer patterns. Compared with the single grain (SG) FE-FinFET, the MG effect induces the variation of FE-FinFET transfer characteristics in both electrostatics and drive-currents. The individual effects of the FE/DE ratio and FE grain orientation on the key electrical FoM fluctuations of MG FE-FinFETs are then investigated, respectively. When $R_{\text{crit}} = 3$ nm or $\sigma_\theta = 25°$ (R_{crit} and σ_θ are parameters to describe the variation of FE/DE ratio and grain orientations), the statistical variability will be comparable to traditional sources.

Physical mechanism analysis. The electrostatic potential

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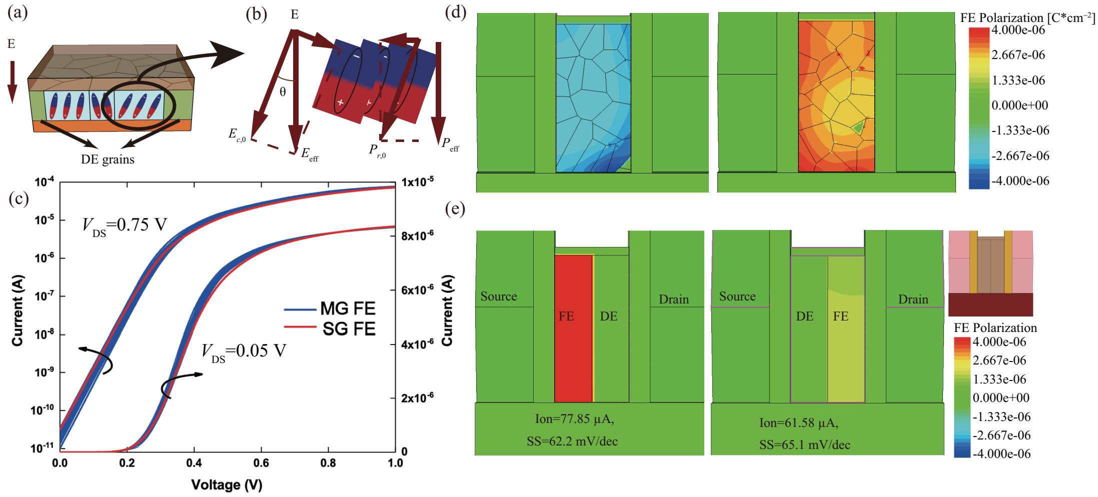

Figure 1 (Color online) (a) MG FE film schematic with different grain shapes, phases, and orientations. (b) Detail schematic of an FE grain's electric field and polarization with an angle (θ) between grain orientation and electric field. (c) The transfer characteristics of SG FE-FinFET and 100 MG FE-FinFETs with different FE layer patterns. (d) The polarization profiles of FE layers on both sides of the fin. The green regions represent the DE-phase grain, while the nonuniform FE polarization results from FE grain orientation variation. The FE layers on both sides are polarized toward or outward from the fin. (e) Two extreme cases of FE polarization with only two grains of FE/DE in opposite positions, with $V_{\rm DS} = 0.75$ V.

distribution of the channel surface and the polarization distribution of the FE gate are analyzed to investigate the physical mechanism by which the MG FE gate layer introduces device-to-device variation into FE-FinFET performance, as shown in Figures 1(d) and (e). The following conclusion can be drawn: The coupling of the ratio of FE/DE and the orientation of FE grains with the spatial distribution of grains leads to the statistical variability of MG FE-FinFETs. The extreme grain distribution, in particular, would result in extreme electrical characteristics. Indeed, for the small dimension FinFETs, not only the average effect will decrease, but the coupled voltage of $V_{\rm D}$ on the FE gate layer will exacerbate the variability induced by the polycrystalline FE gate. The voltage-amplification effect of the FE gate will be stronger than in the opposite case when the FE grains are distributed near the source terminal.

Conclusion. In conclusion, this study proposed a physical MG FE model to describe the polycrystalline FE HfO_2-based film, as well as the modeling method details were also presented. The MG FE model, when combined with the modified L-K model, was successfully introduced to a 7 nm MG FE-FinFET, exhibiting the negative-capacitance voltage-amplification variation effect. The statistical variability of FOMs induced by FE/DE ratio and FE grain orientations is described, which will be comparable with traditional sources when $R_{\rm crit} = 3$ nm or $\sigma_\theta = 25°$. By the analysis of FE polarization and electrostatic potential, the respective effects of the polycrystalline FE layer on the performance of FE-FinFETs are discussed in terms of irregular grains, FE/DE partitioning, and FE grain orientations. With a reduced averaging effect for small dimension FE-FinFETs, the device-to-device variation induced by FE/DE ratio and grain orientation becomes more prominent. In particular, due to the existence of parasitic capacitances at the drain terminal, drain potential induced lateral field can influence the polarization of FE grains, therefore exacerbating the FE polycrystalline effect. Without specific assumptions of the presented model, the conclusion is generic for both memory and logic FE-FET using the state-of-the-art process node.

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Supporting information Appendix A-C. The supporting information is available online at info.scichina.com and link.springer.com. The supporting materials are published as submitted, without typesetting or editing. The responsibility for scientific accuracy and content remains entirely with the authors.

References

1 Khan A I, Keshavarzi A, Datta S. The future of ferroelectric field-effect transistor technology. Nat Electron, 2020, 3: 588–597
2 Cheema S S, Kwon D, Shanker N, et al. Enhanced ferroelectricity in ultrathin films grown directly on silicon. Nature, 2020, 580: 478–482
3 Krivokapic Z, Rana U, Galatage R, et al. 14 nm ferroelectric FinFET technology with steep subthreshold slope for ultra low power applications. In: Proceedings of IEEE International Electron Devices Meeting (IEDM), 2017. 11–14
4 Lederer M, Kämpfe T, Olivo R, et al. Local crystallographic phase detection and texture mapping in ferroelectric Zr doped HfO_2 films by transmission-EBSD. Appl Phys Lett, 2019, 115: 222902
5 Lin Y-K, Kao M-Y, Agarwal H, et al. Effect of polycrystallinity and presence of dielectric phases on NC-FinFET variability. In: Proceedings of IEEE International Electron Devices Meeting (IEDM), 2018. 1–4
6 Tanemura M, Ogawa T, Ogita N. A new algorithm for three-dimensional Voronoi tessellation. J Comput Phys, 1983, 51: 191–207
7 Tang Y-T, Su C-J, Wang Y-S, et al. A comprehensive study of polymorphic phase distribution of ferroelectric-dielectrics and interfacial layer effects on negative capacitance FETs for Sub-5 nm node. In: Proceedings of IEEE Symposium on VLSI Technology, 2018. 45–46