

A two-dimensional threshold voltage analytical model for metal-gate/high- k /SiO₂/Si stacked MOSFETs*

Ma Fei(马飞)[†], Liu Hong-Xia(刘红侠), Fan Ji-Bin(樊继斌), and Wang Shu-Long(王树龙)

*Key Laboratory of the Ministry of Education for Wide Band-Gap Semiconductor Material and Devices,
School of Microelectronics, Xidian University, Xi'an 710071, China*

(Received 6 January 2012; revised manuscript received 15 May 2012)

In this paper the influences of the metal-gate and high- k /SiO₂/Si stacked structure on the metal-oxide-semiconductor field-effect transistor (MOSFET) are investigated. The flat-band voltage is revised by considering the influences of stacked structure and metal-semiconductor work function fluctuation. The two-dimensional Poisson's equation of potential distribution is presented. A threshold voltage analytical model for metal-gate/high- k /SiO₂/Si stacked MOSFETs is developed by solving these Poisson's equations using the boundary conditions. The model is verified by a two-dimensional device simulator, which provides the basic design guidance for metal-gate/high- k /SiO₂/Si stacked MOSFETs.

Keywords: metal-gate, high- k , work function, flat-band voltage, threshold voltage, metal-oxide-semiconductor field-effect transistor

PACS: 73.40.Qv, 73.40.Ns, 73.30.+y

DOI: 10.1088/1674-1056/21/10/107306

1. Introduction

With the size of a MOSFET scaling down to a sub-45 nm node, metal-gate/high- k technology has been recognized as a key process of transistor fabrication.^[1] Metal and high- k dielectrics have replaced poly-Si and SiO₂ as the gate materials. Compared with the metal-oxide-semiconductor field-effect transistor (MOSFE) fabricated by poly-gate/SiO₂ technology, the high- k MOSFET has a small gate leakage current with an increased physical thickness of the gate dielectric.^[2] The metal-gate materials do not react with high- k materials, and the sheet resistance is reduced. There is no gate depletion effect in the poly-gate material.^[3] The metal-gate/high- k technology has become a promising candidate for the next generation MOSFETs. In order to improve the electrical properties of the metal-gate/high- k /Si stacked MOSFETs, it is necessary to introduce a thin interlayer of SiO₂ between the high- k dielectric and silicon.^[4]

The threshold voltage of a MOSFET with a single high- k gate dielectric layer has been studied widely.^[5–7] However, the threshold behaviour of

the metal-gate/high- k /SiO₂/Si stacked MOSFET is rarely involved. The metal-gate and high- k /SiO₂ stacked structure can cause a new threshold voltage shift. The most direct expression of this threshold voltage fluctuation is the influence of charges at the high- k /SiO₂/Si interface and the metal work function fluctuation on the flat-band voltage. In this paper, considering the effect of the metal-gate/high- k /thin-oxide stacked structure on the flat-band voltage, a model of channel potential is obtained by solving the two-dimensional (2D) Poisson's equation, and the threshold voltage analytical model of a metal-gate/high- k /SiO₂/Si stacked MOSFET is developed. The analytical model is verified by using the 2D device simulator ISE-TCAD.

The rest of this paper is organized as follows. In Section 2 the effect of the stacked metal-gate/high- k /SiO₂/Si structure on the MOSFET is studied. In Section 3 the threshold voltage model of the metal-gate/high- k /SiO₂/Si stacked MOSFET is derived. In Section 4 the results of the threshold voltage model obtained in Section 3 are discussed. Finally, the conclusion is presented in Section 5.

*Project supported by the National Natural Science Foundation of China (Grant Nos. 60936005 and 61076097), the Cultivation Fund of the Key Scientific and Technical Innovation Project, Ministry of Education of China (Grant No. 708083), and the Fundamental Research Funds for the Central Universities (Grant No. 20110203110012).

[†]Corresponding author. E-mail: flyinghorse-100@163.com

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2. A metal-gate/high- k /ultrathin-SiO₂/Si stacked MOSFET

The schematic structure of a metal-gate/high- k /SiO₂/Si stacked n-channel metal-oxide-semiconductor field-effect transistor (nMOSFET) and the coordinates used in the solving process are shown in Fig. 1.

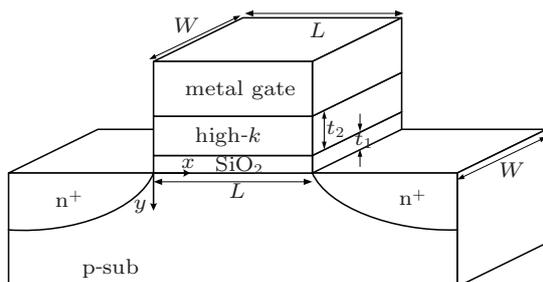


Fig. 1. Schematic structure of a metal-gate/high- k /SiO₂/Si stacked nMOSFET.

A thin oxide layer, high- k dielectric material and metal gate are deposited on the substrate, sequentially. A three-layer sandwich structure is formed. The W and L are gate/channel width and length, respectively. The t_1 and t_2 are the physical thickness values of the oxide and high- k dielectric layer, respectively. The x axis is in the lateral channel direction and y axis is in the direction perpendicular to the channel.

2.1. Fluctuation of the metal-gate work function

The metal work function is defined as the minimum energy required for removing an electron from the Fermi level of a metal material to the vacuum level and making it a free electron. When the metal becomes the primary gate material in advanced CMOS technology, there is a new source of random variation due to the dependence of the work function on the orientation of the metal grain.^[8] It has also become another factor which causes threshold voltage fluctuation.

From Fig. 1 we can see that the gate area is $W \times L$ and it contains many metal grains for a given material. The work function of each grain is a function of its orientation, which is not controllable during the growth period. Hence, the orientation of each grain is determined randomly.^[9] It is known that metal grains usually grow up to a few nanometers in size under temperatures normally used in integrated circuit fabrication. Since the gate dimensions are in the order of a few tens of nanometers, it is expected that the gate contains a small number of grains. So the metal gate work function should be modeled as a probabilistic distribution rather than a deterministic value.^[10] Table 1^[11] shows the physical properties of some metal nitrides of the metal gate. Where titanium nitride (TiN) and tantalum nitride (TaN) are used for n-channel MOS (NMOS) devices, tungsten nitride (WN), and molybdenum nitride (MoN) are used for p-channel MOS (PMOS) devices.

Table 1. Physical properties of different metal nitrides as metal gates.^[11]

Materials	Orientation	Probability	Work function/eV	Grain size/nm
TiN	$\langle 100 \rangle$	60%	4.6	4.3
	$\langle 111 \rangle$	40%	4.4	
TaN	$\langle 100 \rangle$	50%	4.0	7
	$\langle 200 \rangle$	30%	4.15	
	$\langle 220 \rangle$	20%	4.8	
WN	$\langle 111 \rangle$	65%	4.5	10
	$\langle 200 \rangle$	15%	4.6	
	$\langle 220 \rangle$	15%	5.3	
	$\langle 311 \rangle$	5%	4.2	
MoN	$\langle 110 \rangle$	60%	5.0	17
	$\langle 112 \rangle$	40%	4.4	

According to the aforementioned results, we could conclude that the work function induced threshold voltage fluctuation is affected by the gate area, grain size, and the gate material. Yu *et al.*^[1] proposed an analytic formula to describe the effect of work function fluctuation on threshold voltage fluctuation,

However, there is a negative flat band shift when the equivalent oxide thickness is reduced to 2 nm.^[17] When the oxygen diffuses through the gate dielectric, O exits in O²⁻ species and diffuses via an exchange with the lattice oxygen in the high-*k* layer.^[18] Some O²⁻ form metal-O-Si bonds at the high-*k*/SiO₂ interface, and the others are converted into Si=O dipoles at the SiO₂/Si interface. Si atoms have partial positive charges and O atoms are partially negatively charged. These dipoles produce the electric field as shown in Fig. 3, which causes a negative V_{fb} shift. If the thickness of the SiO₂ layer is larger than the O²⁻ diffusion length, fewer dipoles are converted at the SiO₂/Si interface and thus produce a smaller electric field. Hence, a V_{fb} shift shows that it is closely related to the thickness of the SiO₂ layer. The V_{fb} shift can be calculated as follows:^[19]

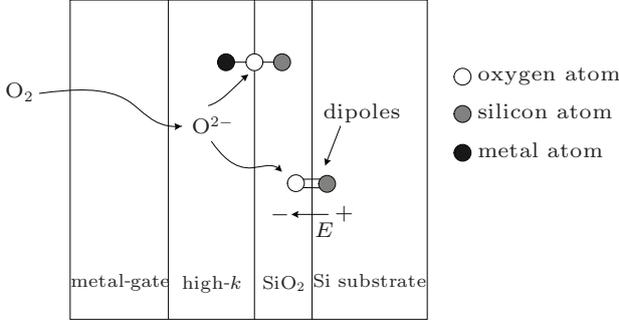


Fig. 3. Diffusion of O into SiO₂ layer from the high-*k* layer, forming dipoles with Si.

$$\Delta V_{fb} = \alpha \exp\left(\frac{-t_1^2}{\beta}\right), \quad (10)$$

where α and β are fitting parameters related to process temperature, the values of α and β are 700 and 25, respectively, and t_1 is the thickness of the interface oxide layer. When t_1 decreases to a certain value, ΔV_{fb} begins to increase rapidly. Considering the effect of dipoles, the flat-band voltage can be written as

$$V'_{fb} = V_{fb} + \Delta V_{fb}. \quad (11)$$

3. Derivation of the threshold voltage model

Neglecting the mobile carriers in the channel depletion region, the 2D Poisson's equation in the channel region can be written as

$$\frac{\partial^2 \varphi(x, y)}{\partial x^2} + \frac{\partial^2 \varphi(x, y)}{\partial y^2} = \frac{qN_A}{\varepsilon_{si}}, \quad (12)$$

$$0 \leq x \leq L, \quad 0 \leq y \leq y_d,$$

where $\varphi(x, y)$ is the 2D potential distribution in the channel, $y_d = \sqrt{4\varepsilon_{si}\varphi_g/qN_A}$ is the width of the depletion region in the substrate, N_A is the doping concentration of the substrate, and ε_{si} is the dielectric permittivity of the substrate. Using a two-order polynomial approximation, $\varphi(x, y)$ can be written as

$$\varphi(x, y) = \varphi_0(x) + \varphi_1(x)y + \varphi_2(x)y^2. \quad (13)$$

To solve the parabolic function, the boundary conditions are shown as follows.

(i) At the SiO₂/Si interface ($y = 0$), the 2D surface potential distribution can be written as

$$\varphi(x, 0) = \varphi_0(x). \quad (14)$$

(ii) The electric flux (displacement) at the SiO₂/Si interface ($y = 0$) is continuous, i.e.

$$\left. \frac{d\varphi(x, y)}{dy} \right|_{y=0} = \frac{\varepsilon_{ox}}{\varepsilon_{si}} \frac{\varphi(x, 0) - V_{gs} + V'_{fb}}{EOT}, \quad (15)$$

where $EOT = t_1 + EOT_h = t_1 + t_2\varepsilon_{ox}/\varepsilon_h$; ε_{ox} and ε_h are the dielectric permittivity of SiO₂ and the high-*k* dielectric, respectively; V_{gs} is the gate-to-source bias voltage; V'_{fb} is the revised flat-band voltage.

(iii) At the depletion edge ($y = y_d$), the boundary conditions are shown as follows:

$$\begin{cases} \varphi(x, y_d) = V_{bs}, \\ \left. \frac{d\varphi(x, y)}{dy} \right|_{y=y_d} = 0, \end{cases} \quad (16)$$

where V_{bs} is the substrate voltage, while the substrate is grounded, i.e., $V_{bs} = 0$.

The values of the coefficients $\phi_i(x)$ ($i = 0, 1, 2$) in Eq. (13) can be determined using the boundary condition Eqs. (14)–(16). Substituting Eq. (13) into Eq. (12) and setting $y = 0$, the two-order differential equation about $\phi_0(x)$ can be obtained as

$$\frac{\partial^2 \varphi_0(x)}{\partial x^2} - P\varphi_0(x) = Q, \quad (17)$$

where

$$P = \frac{\varepsilon_{ox}}{y_d \varepsilon_{si} EOT}, \quad Q = \frac{qN_A}{\varepsilon_{si}} - \frac{\varepsilon_{ox}}{y_d \varepsilon_{si} EOT} (V_{gs} - V'_{fb}).$$

The solution for Eq. (17) is a simple second-order non-homogenous differential equation with constant coefficients, and it can be written as

$$\varphi_0(x) = A \exp(\lambda x) + B \exp(-\lambda x) - D, \quad (18)$$

where $\lambda = \sqrt{P}$, $D = Q/P$, A and B are the coefficients that can be determined by the following boundary conditions:

i) the surface potential at the source end is

$$\varphi(0,0) = \varphi_0(0) = V_{bi}, \quad (19)$$

ii) the surface potential at the drain end is

$$\varphi(L,0) = \varphi_0(L) = V_{bi} + V_{ds}, \quad (20)$$

where

$$V_{bi} = \frac{kT}{q} \ln \frac{N_A N_D}{n_i^2}$$

is the built-in potential of the drain/source-substrate junction, with N_D being the doping concentration of the source/drain regions and n_i the intrinsic carrier concentration; V_{ds} is the drain-to-source bias voltage.

Based on Eq. (18), the minimum surface potential ($\phi_{0,\min}$) can be determined by $d\varphi_0(x)/dx = 0$. Setting $\varphi_{0,\min} = 2\varphi_g$ ($\varphi_g = (kT/q) \ln(N_A/n_i)$), the corresponding gate voltage V_{gs} is defined as the threshold voltage V_{th}

$$V_{th} = \frac{qN_A y_d EOT}{\varepsilon_{ox}} + V'_{fb} - \frac{-b + \sqrt{b^2 - 4ac}}{2a}, \quad (21)$$

where

$$\begin{aligned} a &= \sinh^2(\lambda L) - 2 \cosh(\lambda L) + 2, \\ b &= [2 - 2 \cosh(\lambda L)](2V_{bi} + V_{ds}) + 4\varphi_g \sinh^2(\lambda L), \\ c &= [2 - 2 \cosh(\lambda L)](V_{bi}^2 + V_{bi}V_{ds}) \\ &\quad + 4\varphi_g^2 \sinh^2(\lambda L) + V_{ds}^2. \end{aligned}$$

4. Results and discussion

According to the aforementioned analysis, we can see that the revised flat-band voltage V'_{fb} is a key parameter of the threshold voltage. From Eq. (11), it can be found that the revised flat-band voltage is composed of two parts (V_{fb} and ΔV_{fb}). The former V_{fb} is caused mainly by the metal work function and charges in the gate insulator layers, and the latter ΔV_{fb} is induced chiefly by dipoles at the SiO₂/Si interface.

Figure 4 shows the dependence of revised flat-band voltage V'_{fb} on the interface oxide thickness t_1 . We keep the total equivalent oxide thickness EOT constant ($=2$ nm), and increase the interface oxide thickness t_1 from 0.1 nm to 1.9 nm (equivalent thickness of the high- k layer $EOT_h = EOT - t_1$). It can be seen from the figure that the flat-band voltage shift ΔV_{fb} decreases as t_1 increases, which is consistent with the result of Eq. (10). With the increase of t_1 , the number of oxygen ions diffusing through the oxide decreases. Fewer dipoles are converted at the SiO₂/Si interface, and a smaller electric field is obtained. However, with the increase of t_1 , V_{fb} increases according to

Eq. (9). So the revised flat-band voltage V'_{fb} decreases at the beginning and then increases.

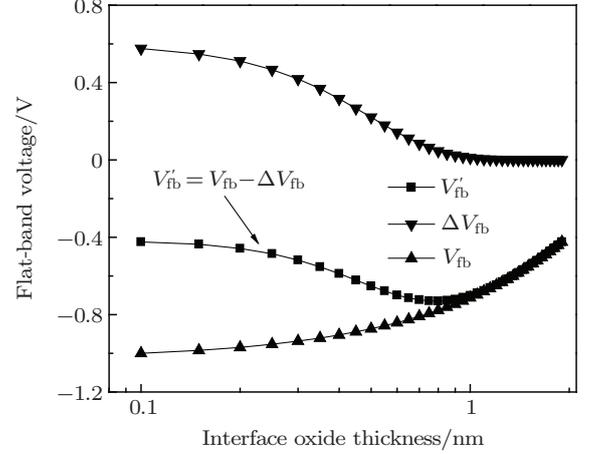


Fig. 4. Variations of the revised flat-band voltage V'_{fb} with an interface oxide thickness t_1 . TiN and HfO₂ are used as the gate material and high- k material, respectively. $N_A = 2 \times 10^{18}$ cm⁻³, $N_D = 1 \times 10^{20}$ cm⁻³, $EOT = 2$ nm, $L = 45$ nm, $V_{ds} = 1.0$ V.

Figure 5 shows the variations of the revised flat-band voltage V'_{fb} with the total equivalent gate oxide thickness EOT . The interface oxide thickness t_1 is kept constant ($=0.5$ nm). Based on Eq. (10), the flat-band voltage shift ΔV_{fb} is the same. The increase of the total equivalent gate oxide thickness EOT means the increase of equivalent high- k thickness EOT_h , and the V_{fb} decreases according to Eq. (9). So the revised flat-band voltage V'_{fb} decreases with the value of EOT increasing.

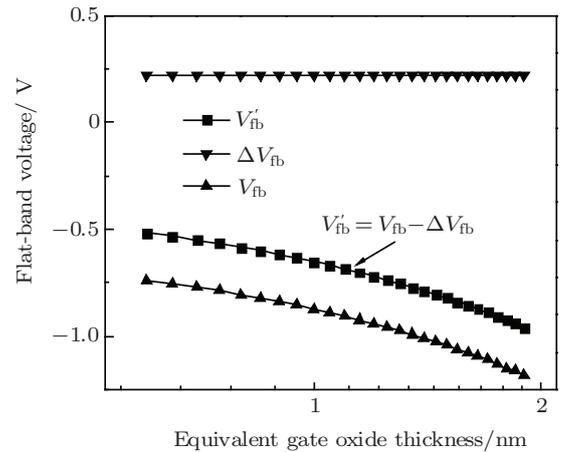


Fig. 5. Variations of revised flat-band voltage V'_{fb} with total equivalent gate oxide thickness EOT . TiN and HfO₂ are used as the gate material and high- k material, respectively. $N_A = 2 \times 10^{18}$ cm⁻³, $N_D = 1 \times 10^{20}$ cm⁻³, $t_1 = 0.5$ nm, $L = 45$ nm, $V_{ds} = 1.0$ V.

In order to verify the proposed analytical threshold voltage model, an nMOSFET with a metal-

gate/high- k /SiO₂ stacked structure is used. The analytical results of the threshold voltage calculated from the model are compared with the numerical results obtained by the 2D device simulator ISE-TCAD. The relationship of the key device parameters and the threshold voltage is analysed.

Figure 6 shows the dependence of the threshold voltage V_{th} on the substrate doping concentration N_A . For the same device structure, doping profile and geometrical dimensions are used in both analytical model and 2D numerical simulations. Good agreement is obtained between the prediction from the analytical model and the 2D numerical simulation results. For nMOSFETs with a constant source/drain region doping concentration N_D , the threshold voltage V_{th} increases with the increase of substrate doping concentration N_A . When the acceptor impurity concentration in the channel region increases, the thickness of the channel inversion layer decreases, and the source to drain current gradually decreases. A larger gate voltage is required to turn on the channel.

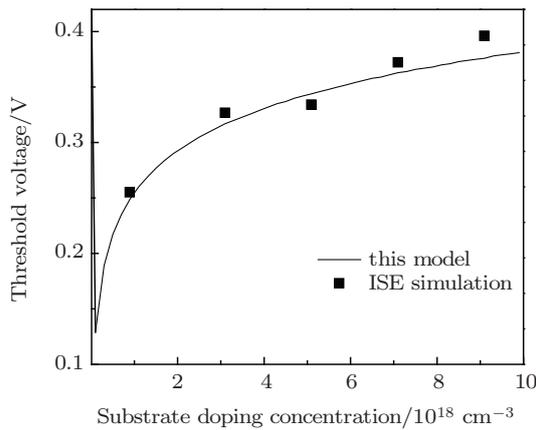


Fig. 6. (colour online) Variation of the threshold voltage V_{th} with substrate doping concentration N_A . TiN and HfO₂ are used as the gate material and high- k material, respectively. $N_D = 1 \times 10^{20} \text{ cm}^{-3}$, $EOT = 1 \text{ nm}$, $EOT_h = t_1 = 0.5 \text{ nm}$, $L = 45 \text{ nm}$, $V_{ds} = 1.0 \text{ V}$.

Figure 7 shows the dependence of the threshold voltage V_{th} on channel length L . For a given channel doping concentration, the threshold voltage V_{th} increases with the increase of channel length due to the reduction in influence of the source and drain junction depletion layers. In other words, with the channel length shrinking, the depletion layer widths of the source and drain region make an effective channel length decrease. The current from source to drain increases, which leads to a lower threshold voltage. It can be seen from the figure that the threshold voltage V_{th} increases with gate length L increasing. The

results derived from the analytical model accord well with the ISE-TCAD simulation results.

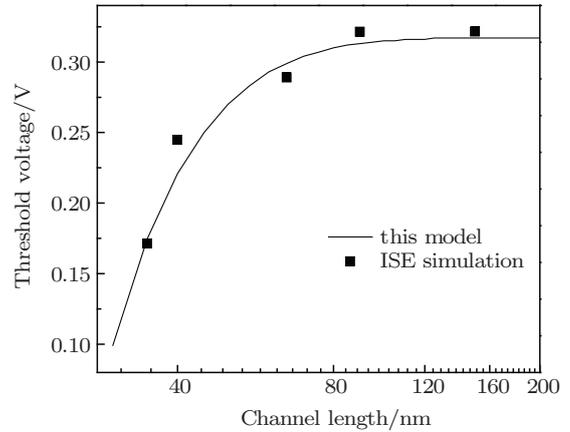


Fig. 7. Variation of the threshold voltage V_{th} with channel length L . TiN and HfO₂ are used as the gate material and high- k material, respectively. $N_A = 2 \times 10^{18} \text{ cm}^{-3}$, $N_D = 1 \times 10^{20} \text{ cm}^{-3}$, $EOT = 1 \text{ nm}$, $EOT_h = t_1 = 0.5 \text{ nm}$, $V_{ds} = 1.0 \text{ V}$.

Figure 8 shows the dependence of the threshold voltage V_{th} on the drain voltage V_{ds} . Similarly to the mechanism for the effect of channel length on the threshold voltage, the threshold voltage V_{th} decreases as the drain voltage V_{ds} increases. When the channel length and doping concentration are fixed, the width of the drain junction depletion layer increases with the drain-to-source bias voltage increasing. The effective channel length decreases, and a lower threshold voltage is obtained. So the threshold voltage decreases with increasing drain voltage. The results obtained from the model agree well with the ISE-TCAD simulation results.

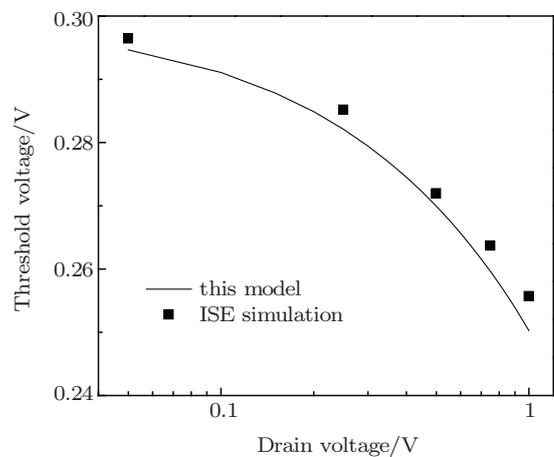


Fig. 8. Variation of the threshold voltage V_{th} with the drain-to-source bias voltage V_{ds} . TiN and HfO₂ are used as the gate material and high- k material, respectively. $N_A = 2 \times 10^{18} \text{ cm}^{-3}$, $N_D = 1 \times 10^{20} \text{ cm}^{-3}$, $EOT = 1 \text{ nm}$, $EOT_h = t_1 = 0.5 \text{ nm}$, $L = 45 \text{ nm}$.

5. Conclusion

In this paper, the metal-gate/high- k /SiO₂/Si stacked structure is presented. The influence of metal-gate and high- k stacks on the flat-band voltage is investigated. The revised metal-semiconductor work function and revised flat-band voltage are obtained. The two-dimensional potential distribution Poisson's equation is developed and also solved using the boundary conditions. A threshold voltage analytical model for a metal-gate/high- k /SiO₂/Si stacked MOSFET is presented, which is consistent with the simulated results.

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