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Beyond CMOS Nanodevices for Adding Functionalities to CMOS

Network of Excellence

WP 1 Nanosensing with Si nanowires

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Deliverable Summary:

Si nanowire FETs (NWTs) are very promising transducers, in particular for label-free sensing and detection of biological species. Nanowires indeed provide a very high sensitivity (S) to many analytes of interest, allowing one to sense biological phenomena with an unprecedented level of precision. However due to the complexity and "multiphysics" nature of the phenomena involved, there is still a lack of understanding of the physics and how design parameters quantitatively impact S. Furthermore, there are little simulation tools and models allowing for the understanding, prediction and co-design of such bio-electronic systems. To address these issues, different partners in the consortium have set upon to build simulation tools adapted for the task. At UCL, a dedicated full quantum microscopic platform has been extended towards the simulation of Si NWT biosensors (NWTBs) scaled close to the technological limit in order to investigate their ultimate sensitivity limit (down to single analyte detection) and physics (first activity). Indeed, although models and experiments have predicted S improvement when scaling the NWTs dimensions down, there is little study of S and physics of nanowires scaled deep down in the nanoscale regime. Furthermore this platform is used as a benchmark for validation of simpler but faster models developed at UCL or by other partners. The second activity developed by Udine, mainly report the adaptation of a commercial TCAD simulator (SDevice) in order to implement the "electrolyte" material. This approach exploits the similarity between the semiconductor equations and the ones describing positive and negative ions. It trades a simplified description of the electrolyte to the advantages of exploiting and leveraging all functions of the TCAD such as, for the silicon part: calibrated mobility models, DC, AC and noise analysis, handling of arbitrary geometries in 2D and in 3D. A first validation of this approach by comparison of UCL and Udine simulations on a benchmark device in air and ionic solution is also reported. It is known and also quantitatively shown in this report (e.g. 1st activity), that ion screening can strongly degrade S. Although the capture of the analyte usually requires to be done in ionic solution, it is possible, if the application allows it, to measure in a post sequence in dry environment, hence getting rid of the ion screening problem. Such an approach is described in the third activity developed by INP Grenoble. They put the effort on using a model system able to retain the main characteristics of the experimental devices presently under fabrication taking advantage of a rather light and handy simulation platform. The aim is to identify general trends to be further compared to experimental ones. Therefore, no attempt has been made here to account for the localized nature of the charge and an equivalent density of charge was used instead. To summarize, the simulation efforts have been devoted to assessing sensitivity with respect to a given charge. This has provided us with a deep understanding of the physics and where lie important design parameters to optimize and challenges to overcome in the transduction part. These simulation tools serve as guideline for setting up experimental conditions and interpreting experimental results of real devices fabricated within the consortium. The missing part that will be developed in the remaining of this project is related to the relation between given analytes in solution and the related charges on the sensor. This implies specific molecule models with shape and charge configurations that can be pH dependent as well as dynamic drift and diffusion equations in order to asses diffusion and hence measurement time.

1. A dedicated simulation platform for the investigation and design of ultimate nanowire-FET biosensors: (UCL)

1.1 Introduction

Si nanowire FETs (NWTs) are very promising transducers, in particular for label-free sensing and detection of biological species [Ham04,Stern07,Li05]. Although models and experiments have predicted sensitivity (S) improvement when scaling the NWTs dimensions down, there is little study of S and physics of nanowires scaled deep down in the nanoscale regime. Furthermore, semi-classical models, such as Drift-Diffusion (DD), are mostly used for simulating transport in such systems [Ham04, Stern07,Li05,Nair07]. Such models do not include quantum effects and are based on macroscopic mobility models. In this work we have used our dedicated quantum simulation platform NANOcore, using full quantum microscopic Non-Equilibrium Green's Functions (NEGF) formalism [Afzalian07, Afzalian11], to investigate the sensitivity and physics of top-down Si NWT biosensors (NWTBs) scaled close to the technological limit, i.e. where S is expected to be the highest (up to single analyte detection) and quantum effects are strong [Afzalian12].

In order to asses whether approaches based on semi-classical models could yield the required precision and what would be their specific transport models requirements at this scale, we also developed within NANOcore quantum corrected macroscopic (QC) DD methods [Ferry93,Baccarani08] and compared the resulting simulation results with NEGF ones. Furthermore a comparison with the TCAD simulator using semi-classical model models adapted to simulate biosensor in electrolyte solution (task done by the Udine partner) has been started.

1.2 Methodology / Networking and collaboration

The system under study is a square cross-section N-doped NWT of side-dimension d_{SI} with an intrinsic channel biased by a bottom gate that also serves as a reference electrode (Fig. 1). The side and top gates are left floating and consist of an oxide layer of equivalent thickness EOT on which dielectric selfassembled monolayers (SAM) can potentially be added for increasing the selectivity of the NWT. This affinity-based layer is supposed to be flat and homogenous of thickness t_{SAM} and to have a relative dielectric permittivity ε_{rSAM} . On the top gate, centered at half the length and width of the channel, an analyte of charge z_a.q is placed. In this study, as we are interested to get general trends on the fundamental detection limit of ultra-scaled nanowires, we have used as analyte the smallest detectable unit, i.e. a simple discrete electronic charge. A surrounding media on the top and side of the NWT is considered and taken wide enough (typically from 10 to 100 nanometers) so that the results do not change when further increasing its thickness. We have considered both air and NaCl solution with an ionic concentration cion0. Each ion species i with charge valence zi in the solution is assumed to follow a modified Boltzmann distribution (MBD), which is essentially a Boltzmann distribution modified to include steric effects that become important at large voltage ($\Phi(r)$) through an effective ion diameter d_{si} [Killic07]. For the electronic part, we have used a previously developed Self-Consistent NEGF code to simulate the nanowires [Afzalian07,Afzalian11]. The electronic wave functions are calculated in the Si and surrounding oxides. A (Fast-) coupled mode space ((F)CMS) is chosen as it is much faster than a real space approach, while conserving the required accuracy by preserving the mode coupling in the vicinity of the perturbation potential of the charged analytes. The Hamiltonian is written in the effective mass formalism using NWT diameter-dependent effective masses that are extracted from a sp3d5s* Tight-Binding Hamiltonian [Afzalian07]. Phonon scattering is accounted for within the Born Self-Consistent framework [Afzalian11]. The influence of the analyte and possible ions is directly included in a non-perturbative way through the electrostatic potential that is solved for in the full domain, NWT and surrounding media (Fig. 2).



Figure 1. Schematic of the [100] SOI square cross-section N-type nanowire with floating top and lateral gates (the lateral gates are not shown) and a single analyte on the top gate.

Furthermore, as said above, this platform is used as a benchmark for validation of simpler but faster models developed at UCL or by other partners. Such models can make it easier to compare with fabricated devices (device fabricated within the consortium for which UCL played a role in defining mask structures and will perform the electrical characterization) whose dimensions may be too big to simulate with a full quantum approach.



1.3 Results and discussion / Perspectives

Figure 2. XY-plots in the Z-plan cutting across the middle of the NWT with a single negative charge on the top gate and a 60nm surrounding. A) Potential in air media at V_G=0.7V. B) Potential in NaCl 1mM ionic solution media at V_G=0.7V. C) Carrier concentration (electrons, ions) at V_G=-0.4V. L=20nm. S/D extensions: L_S=8nm L_D=12nm, V_D= 0.7V, doping N⁺=10²⁰cm⁻³. Oxide: EOT=0.5nm. t_{SAM}=0nm. T=300K.

d _{si}	L	s.	S+	$t_{SAM}(nm)$	media
(am	(nm)	(mV/q)	(mV/q)	(s _{rSAM} =2.3)	
)					
2	20	-145	58	0	air
3	20	-97	68	0	air
4	20	-61	56	0	air
6	20	-84	86	0	air
3	60	-69	11	0	air
3	100	-16	3	0	air
2	20	-32	29	0	water c _{iono} =0
2	20	-20	10	0	water c _{iono} =1mM
2	20	-1	1	0	water
					c _{tono} =100mM
2	20	-3	3	2.5	waterc _{iono} =1mM
2	20	-1	1	5	water c _{iono} =1mM
3	20	-65	62	2.5	air

Table 1. Simulated NWT Sensitivity to a positively S_+ or negatively S. charged analyte for various device parameters with EOT= 0.5 nm. The sensitivity is expressed as the $V_{\rm TH}$ shift extracted at $I_{D,0q}{=}10^{-7}$ A/µm normalized by the number of charge.

The fundamental detection limit of ultra-scaled NWTBs is studied with a quantum microscopic approach (Table 1). For negatively charged analytes, an N-doped NWT is more sensitive and gets less sensitivity degradation when increasing channel length (by reciprocity a P-doped NWT will be more sensitive to detect positively charged analytes). Our results predict S in the order of tens to hundreds of mV/q in dry (air) or low ionic solution environments, which hints at single charge/analyte detection. In this case also, the design space in terms of channel length and cross-section to get such a high

sensitivity is not too severe compared to today's fabrication capabilities. However, S rapidly drops down to the mV/q range in typical ionic solution and SAM conditions (Table 1 and Fig. 3). This translates in I_D variation of a few percent or less. In this case the design space to get single charge detection is quite narrow and in particular having the charge as close as possible to the surface of the sensor and find adequate way to get rid of ion screening is crucial to enhance the sensitivity.



Figure 3. Simulated V_{TH} shift compared to the 0q case for a charged analyte with z_a =-1 and +1, extracted at $I_{D,0q}$ =10⁻⁷ A/µm in solution A) in function of c_{ion0} with t_{SAM} =0nm , B) in function of t_{SAM} with c_{ion0} =1mM. d_{SI} =2nm, V_D =0.7V. EOT=0.5nm. ϵ_{rSAM} =2.3.

Finally we have compared microscopic quantum NEGF and macroscopic quantum corrected DD methods to investigate the sensitivity (S) of ultimately scaled Si nanowire FET biosensors (NWTBs). Our dual approach enables us to draw important conclusions on the origin of the threshold voltage shift that directly relates to sensitivity and on NWTBs specific transport models requirements. We show that, in ultimately scaled NWTBs, S is related to a direct or energy band shift and an indirect or mobility shift. This requires one to develop adequate mobility models when using macroscopic simulations.

2. Customization of a commercial TCAD to handle dielectric screening by the electrolyte (Udine)

2.1 Introduction

The sensitivity of a biosensor is strongly degraded by the dielectric screening of the electrolyte [Nair07]. Unfortunately, the ion concentration in the electrolyte cannot be reduced below the level needed to leave the properties of the target molecules unaffected. In fact, most analytes require a minimum salt concentration. Modelling of dielectric screening is typically based on the solution of the Poisson-Boltzmann equation by means of ad-hoc simulation codes [Pittino12,Yang12], since, available TCAD tools are not equipped to model the electrolyte and are inefficient and sometimes even inaccurate when it comes to simulate small biomolecules. On the other hand, commercial TCAD tools already have very sophisticated models for the semiconductor material and the capability to handle complex device geometry.

In the framework of Nanofunction project we have thus pursued two complementary approaches:

1) implement the "electrolyte" material into the commercial TCAD simulator SDevice [Sdevice11]; this approach is described in the following and we will see that it trades a simplified description of the electrolyte to the advantages of exploiting all functions of the TCAD;

2) develop an ad-hoc simulator implementing an accurate description of the electrolyte; this approach has been so far applied to nano-electrode based biosensors [Pittino12] and is not reported in this deliverable, that is devoted to nanowires. In the future we plan to add to the ad hoc-code models for the silicon channel in order to handle nanowire type of sensors as well.

2.2 Methodology / Networking and collaboration

We have implemented the "electrolyte material" in SDevice by exploiting the similarity between the semiconductor equations and the ones describing positive and negative ions. The electrolyte is thus described as a semiconductor with zero gap, dielectric constant of $80\varepsilon_0$ at 300K and effective density of states in conduction and valence band:

$$N_C = N_V = N_A c_0$$

where N_A is Avogadro's number and c_0 the ion molar concentration in the bulk of the solution where we have the same number of positive and negative ions. This of course works only for 1:1 electrolytes since opposite charges are described as electron and holes and thus they must have the same charge. For a solution with a given pH:

$$N_{C} = N_{V} = 6.022 \cdot 10^{20-pH} \, cm^{-3}$$

Also, the mobility of the ions is much lower than the electron and hole mobility in semiconductors. However, we report here DC simulations where the electrolyte is at equilibrium and the mobility value does not influences the results. This approach has the advantage of exploiting all the features of the TCAD tools, such as, for the silicon part: calibrated mobility models, DC, AC and noise analysis, handling of arbitrary geometries in 2D and in 3D. The disadvantages are: limited accuracy for small biomolecules, no numerical control on the numerical error, only 1:-1 ionic solutions, no steric effects, no interface effects (i.e. chemical reactions at the SiO2/solution interface). We recently became aware that a very similar approach has been published in [Chung12]; this publication proves that the proposed solution is at the state of the art.

Mutual comparison between our approach and the one employed by partner UCL is reported below.

2.3 Results and discussion / Perspectives

We have applied this approach to various case studies such as pH meters and nano-bio-sensors. We have mainly considered planar structures with large width that can be simulated with a 2D grid. However, the approach is also capable of handling 3D structures as demonstrated by the comparison with the model by the UCL partner. A sample result is reported in Figure 4 as the threshold voltage variation of double gate pH sensors. The slope of the V_{th} variation on the fluid gate (the electrolyte is in between the front oxide and the fluid gate on top) is essential 59meV/pH, whereas the one on the back-gate increases roughly as the ratio of the fluid and back-capacitances.



Figure 4. Simulated threshold voltage variation (w.r.t. pH=7) as a function of the pH of the electrolyte. Devices with L=1um, $T_{\rm Si}{=}30 {\rm nm}\ N{=}10^{15} {\rm cm}^{-3}$ and different front- and back-oxide thicknesses.



Figure 5. Simulated threshold voltage for a MOSFET with charged molecules on top of the SiO2 layer. Molecules are simulated as cubes of $5x5x5nm^3$ with 2.5q charge and $2.5\varepsilon_0$. The electrolyte is above the layer of bio-molecules.

Another example is in Figure 5, reporting the threshold voltage of a MOSFET in the presence of biomolecules on top of the SiO₂ gate oxide, simulated as uniform layer with uniform charge density. At high pH (low ion concentration) the threshold voltage shift induced by the bio-molecules is significant, but it reduces as the pH is reduced, due to dielectric screening. However, at low pH (high ion concentration) even if screening is very strong, we see a difference in V_{th} due to a purely electrostatic effect: the dielectric constant of the molecules is $2.5\varepsilon_0$ vs. 80 ε_0 for water.

The effect of the channel doping on the sensitivity of an SOI biosensor is analyzed in Figure 6: if the doping is large, the channel conductance is hardly modulated by the charge associated to the biomolecules.

In summary, we have seen that the implementation of the electrolyte into a commercial TCAD lead to a very versatile modeling tool that can be applied to a large variety of sensor structures and operating conditions. Although we considered here the effect of the bio-molecules on the DC characteristics, the TCAD tools can also perform AC and large signal analysis and are suited to study the possible improvements related to AC readouts at frequency above the electrolyte cut-off frequency that may overcome the limitations due to Debye screening and provide better sensitivity w.r.t. reading the DC conductance. About the limitation of the approach presented here, we are extending our simulator for nano-electrodes to handle nanowires. In such model steric effects and solutions different to 1:1 ions can be handled naturally.



Figure 6. Normalized change in the conductance of a SOI biosensor (Tox=10nm, Tch=100nm, L=10 μ m) as a function of the area density of charge associated to the bio-molecules. The electrolyte with pH=7 is above the layer of bio-molecules. The device is biased at low V_{DS} and the back-gate bias is set to work close to fully depletion in the low doping case. Different dopings in the channel are considered.

In order to check the accuracy of the method, comparison with the UCL NEGF simulator presented in activity 1 has been started. A first template device of 5x5 nm² crossection has been chosen as a trade-

off to keep quantum effect not too strong and keep simulation time for the quantum simulator fast. A 20nm channel length has been chosen since results from the UCL partners have shown that in such device the channel is too short for strong velocity overshoot phenomena to happen so that a simple drift-diffusion (DD) model with quantum correction (here we used the density gradient (DG) model of the simulator) could fairly reproduce the transport part. As can be seen in Fig. 7 a raisonable agreement can be achieved both in air and ionic solution without analyte. The case with analyte is currently under investigation.



Figure 7. $I_D(V_G)$ characteristic of the 5x5 nm² Si N-NWT given by NEGF and the commercial TCAD using a DD-DG model in air (left) and in a 10mM ionic NaCl solution (Right). L=20nm, intrinsic channel doping, V_D =0.7V. DD-DG TCAD include velocity saturation with default parameters for Si.

3. Simulation of the electrical response of Silicon Nanowire DNA sensors in a dry environment. (Grenoble-INP)

3.1 Introduction

Field Effect sensors in which the channel is in the form of a chemically synthesized SiNW or a carbon nanotube [Star03,Kong00] have demonstrated unprecedented performances in terms of sensitivity and specificity. Device sensitivity depends on intrinsic parameters such as NW doping level, length, section and the detailed electrostatics of the complete system taking into account the surrounding medium [Nair07]. Indeed, nanowire biosensors need to be operated for detecting biological species in non homogeneous samples like, for instance, human serum. Biological fluids can pose severe limitations on the ultimate sensitivity since they have a high ionic strength which can effectively screen the electrical charges on the biomolecules to be detected. However, it has been shown that hybridization of biomolecules to their target DNA probes was still detectable after drying [Dechoux07]. Thus, Grenoble-INP simulation objectives in WP1 for the period of interest have been the simulation of the electrical response of the DNA nanowire sensors in a dry environment with the precise scope to find a set of parameters enabling the maximization of device sensitivity.

3.2 Methodology / Networking and collaboration

The device simulated is a SiNW functionalized with DNA capture probes grafted on the silicon oxide external coating to provide selectivity to the target molecules present in the sample solution. Hybridization of the target DNA strands with the DNA probes grafted on the nanowire results in a

change in the external charge at the surface of the nanowire. In dry environment, due to the absence of screening, it can be considered that the external charge on each DNA probe is doubled once hybridized with its complementary strand.

The sensing element can be conceived either in the form of a NW array or as a stand-alone device. Stand-alone nanowires have the advantage of allowing precise correlation between physical and electrical parameters. However, for practical applications, fabrication in arrays is mandatory to increase sensing surface and allow target molecules to be captured effectively. Thus experimental devices have been designed mainly with array structures. Varying pitches have been designed in order to check analyte depletion effects and influence on target molecules capture experimentally. However, for the simulation of the dried system, this may be simply viewed as a variation in the external charge at the NW surface. Influence of variability between nanowires in a single array can be estimated from variations in geometry. Thus, simulations have been carried out for individual nanowires.

The principal objective is then to simulate device performances by varying important physical parameters of the sensors which are directly accessible by the standard CMOS fabrication tools and to verify those predictions by actual measurements on samples presently under fabrication within the consortium. The activity of Grenoble-INP is then not only related to the theoretical understanding but also to the validation of the physical concepts governing the sensing mechanisms through a detailed electrical characterization. To this end we put the effort on using a model system able to retain the main characteristics of the experimental devices presently under fabrication taking advantage of a rather light and handy simulation platform. We simulated device electrostatics by solving Poisson equation using a finite element analysis mathematical approach in the 2D SiNW section and studied its dependence to various design parameters. No attempt has been made here to account for the localized nature of the charge and an equivalent density of charge was used instead. Validation of the modelling approach will be supported by electrical characterization, both in liquid and dry environment. In order to support this study, Grenoble-INP has thus contributed to several mask designs for the realization within the consortium of test devices (nanowires fabricated by e-beam (AMO) and STL (KTH) methods) allowing above mentioned effects to be studied experimentally.

3.3 Results and discussion / Perspectives



Figure 8. Representation of the bidimensional mesh on which the Poisson equation is solved. The equilibrium carrier densities are calculated in the Silicon region (orange domain) given the boundary conditions assigned on the external sensing surface (light blue domain), at the Si/SiO₂ interface and at the back gate.

The sample geometry (Figure 8) under study is a SiNW fabricated following a conventional top-down process flow on a Silicon-On-Insulator (SOI) substrate. The geometries of interest are those directly comparable to the physical dimensions of the samples processed by other partners of the Nanofunction consortium for a direct comparison between experiment and theory.

The functionalization process results in a thin oxide layer around the SiNW. From an electrical point of view, the probe DNA strands are represented by their charge. The distributed external charge is calculated as a function of the number of bases per strand and of the density of grafted strands. From data obtained within Grenoble-INP about functionalization studies (D1.3), the equivalent charge for the model DNA strands used experimentally was taken of the order of 10^{12} cm⁻². The system is considered to be in air. The 2D electrostatic potential V(x,y) is obtained from the solution of the Poisson equation with boundary conditions assigned on the boundaries of the device. The boundary conditions include the external density of charges, back gate voltage, and in addition to most published results, interface states at the silicon/ silicon oxide interface. Quantum effects were accounted for by a corrective factor following Hansch's approximation [Hansch89]. The equilibrium carrier density is calculated as a linear carrier density by integration across the nanowire section. It changes from n₀, before hybridization, to n₁, after hybridization. However, the change in carrier density is expected to be strongly influenced by back gating on one side, and by the presence of interface states that may partially screen the change in external charge on the other side.

Back gating is obtained by applying a substrate bias to the SOI wafer. The net effect of the hybridization is the sizeable change of the threshold voltage for the electron channel. This is shown in Figure 9 where the linear density of electrons is plotted as a function of the back-gate potential. The assumption about exact charge distribution plays a negligible role, as shown in Figure 10. This is a consequence of Gauss theorem, at least in the limit of a dry environment configuration and as long as the charge can be considered as distributed. More precise simulations would require 3D simulations to be performed in order to account for localization effects.



Figure 9. Simulated carrier densities at equilibrium as a function of the external gate-voltage for three different surface charge values. The negative charged DNA probes shift the threshold voltage for electron accumulation towards more positive values (black curve). This effect is further enhanced after the hybridization of the complementary strand (blue curve). The simulated curves correspond to a nanowire of width W=20nm and height h=15 nm.



Figure 10. Simulated carrier densities at equilibrium for a SiNW sensor according to the model used to distribute the external charge. The solid and dotted curves represent the linear density of electrons before and after hybridation, respectively. In red, the DNA charges are modeled by a density of charge distributed over the anchoring surface. In blue, the same density of charge is distributed in two layers separated by 70nm. W=20nm, h=15nm. Density of DNA probes: $2 \times 10^{12} \text{ cm}^2$.





Figure 11. Calculation of the device sensitivity defined as the percentage variation of the conductance normalized to the number of d hybridyzed strands. The peak sensitivity is always in the subthreshold regime and progressively increases as the device section shrinks. In the graphs w and h are the device width and height, respectively. In the inset is shown the calculated sensitivity when the system can be approximated as a thin film.

Figure 12: device sensitivity in the presence of an interface trap density at the interface between the nanowire siliobn core and its functionalization oxide. The external charge density is N_{ext} =-10¹²cm⁻².

Figure 11 shows the calculated sensitivity of the sensor as a function of gate voltage for different geometric parameters such as the width and height of the nanowire. Nanowire sensitivity was calculated as the percentage variation of channel conductance Δ G/G normalized to the number of the hybridized strands on the sample surface. It was thus calculated in units of length/electron. Maximum sensitivity was obtained in the subthreshold region. This puts in light the importance of monitoring back gate voltage in a FET detection sensing scheme. Sensitivity increases progressively as device dimensions shrink. The influence of nanowire thickness increases as NW width decreases. The inset displays the results obtained with a thin-film like configuration (wide structures). The NW configuration improves sensitivity by about a factor 10. For instance, starting from a 15nm SOI thick layer, sensitivity rises from 0.2 nm/electron to 2 nm/electron when the sensing element width decreases from wide (thin-film configuration with widths above 500nm) to 20 nm nanowires. However, this should be put in balance with the fact that the capture area is smaller in the nanowire configuration, depending on the pitch used. An example of account for interface states is shown in Figure 12. It was found that interface states have no effect on the maximum sensitivity. They simply reduce the voltage window where this sensitivity can be obtained.

To conclude, a simple simulation platform was developed for rapid evaluation of nanowire sensitivity accounting for its geometry, back gate voltage, external density of probe DNA strands and interface states. This platform will be available to give theoretical evaluation of the sensitivity that can be expected from fabricated sensors after drying. It can be extended in the future for studying more complex systems such as nanowire arrays, in order to evaluate possible cross-talk phenomena that could arise at ultra small pitch, especially in the case of long DNA strands in dry environment. In such a case, the distribution of the charge along the nanowire may matter.

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