Predictive Analysis of Negative Bias Temperature Instability Using Data-Driven Machine Learning Techniques

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Abstract

Negative Bias Temperature Instability (NBTI) is a major reliability risk in current CMOS technology, affecting threshold voltage shift, performance deterioration, and long-term device longevity. Accurate prediction of NBTI-induced aging is becoming increasingly difficult because to technological scalability, process variability, and complicated stress-recovery behaviors those conventional physics-based models cannot fully represent. This research proposes a data-driven machine learning methodology for predicting NBTI degradation and estimating semiconductor device lifetimes. The suggested method is based on experimentally recorded and simulated NBTI stress data, which includes essential operating parameters such as temperature, bias voltage, stress time, and recovery conditions. Multiple supervised learning models, including regression-based and ensemble approaches, are used to predict threshold voltage shift and device longevity. Standard error metrics and cross-validation are used to evaluate model performance, and the results show that it outperforms traditional analytical models. Feature significance analysis is used to identify prominent elements impacting NBTI degradation, hence improving model interpretability and reliability evaluation. The results show that machine learning models efficiently capture the nonlinear correlations found in NBTI aging phenomena and generalize well across different stress circumstances. The proposed methodology provides rapid and accurate lifetime prediction, making it ideal for early-stage design reliability assessment and adaptive aging-aware circuit optimization. This paper presents a scalable and efficient solution for NBTI analysis in advanced semiconductor technologies by integrating data-driven learning and reliability modeling.

Keywords:NBTI; Degradation; Reliability; Machine Learning.

I. Introduction

In recent days an increased vulnerability towards reliability mechanism has been noticed with respect to increase in advanced CMOS nodes technology scaling. In PMOS devices, NBTI has turned out as a significant aging phenomenon. Negative Bias Temperature Instability (NBTI) has been extensively studied for its impact on performance degradation and lifetime reduction in deep-submicron CMOS technologies. A threshold voltage shift is observed at an elevated temperature. This is due to the application of a negative biased in the device, which causes interface trap generation and charge trapping at the Si-SiO_2 interface. Such process can be studied with the support of traditional analytical models such as the Reaction-Diffusion (R-D) model. It provides a better theoretical understanding, while it lacks in adaptability to process variations. On the other hand, the latest advances in data-driven techniques have created to scope to enhancement in predictive accuracy using empirical stress data.The proposed work deals with a comprehensive ML-based predictive framework for estimating NBTI. The framework uses various stress parameter such as Stress voltage (V_g), Temperature (T), Stress time (t), Channel length (L) and Oxide thickness (t_{ox}) for estimating NBTI-induced ΔV_{th}.

The following section reviews the progression of NBTI modeling from physics-based analytical models to latest data-driven and machine learning techniques. In specific the approaches such as Physics based modeling of NBTI, Empirical approaches, Semi-empirical approach, Statistical techniques and Machine learning techniques are studied. The trap-generation process at the Si–SiO_2 interface was the fundamental studies done for understanding of NBTI. Followed by that the Reaction–Diffusion (R–D) model, which has been widely adopted as a benchmark for NBTI characterization. H. Reisinger et al. emphasized that the power-law behavior with stress time and also revealed that interface trap generation and hydrogen diffusion control the threshold voltage shift (ΔV_{th}) over time. It was also highlighted that calibrations of multiple physical parameters were required in R–D models [1]. Microscopic trap generation models were the subsequent work proposed by Alam and Mahapatra. In this model both bias and temperature acceleration was taken into consideration. Interface oxide traps and capture emission dynamics have been incorporated in this model. This ensures better correlation with experiments under certain stress ranges [2].

Based on empirical parameters, TCAD tools have enhanced physical models such as tunneling effects, trap and charge generation. TCAD tools have turned out to be computationally expensive though the TCAD simulations offer high reliability. Apart from expensive nature, the simulation demands for a detailed process specific calibration [3]. Similarly, various studies have been done using Empirical and Semi-Empirical Approaches. Due to limitations of pure physics models, empirical formulations on Power-Law Time Dependence use empirical power-law fitting to describe ΔVth evolution $\Delta V_{th}=A\cdot t^{n}$, where A and n are fitting parameters. This approach offers simplicity but lacks generalization beyond the fitted data [4].In **t**emperature acceleration models, **t**emperature acceleration factors are often modeled using Arrhenius relationships. These models capture thermal effects but still struggle with multi-parameter interactions present in modern nanoscale technologies [5].

II. Literature survey

As the technology scales down, the complexity to model device characterization becomes too difficult. Recently, many studies have been evolved by employing Statistical and Machine Learning techniques. Support Vector Regression (SVR) and polynomial regression are few techniques to address such complex model. Similarly, another such attention grabbed method is data-driven method for reliability prediction. These methods have the ability to model complex, non-linear interactions without explicit physical equations and hence it has been applied to model NBTI degradation. The implementation handles non linearity and thus shows improvements over simple empirical models [6]. Robustness to noise and ability to model feature interactions have been demonstrated by Random Forest algorithms. This algorithm yields better results in reliability prediction. Also, it is been employed for predicting Hot Carrier Injection (HCI) and Electromigration [7]. Device aging prediction is done using feedforward neural network and Artificial Neural Networks (ANNs) provide powerful non-linear mapping capabilities. Similalry,ANN can also used for estimating the device degradation physics with limited data [8], [9]. Emerging deep learning models such as Convolutional Neural Networks (CNNs) and Long Short-Term Memory (LSTM) networks have been explored for time-series reliability data. These architectures can learn temporal dependencies and capture aging trends more effectively than shallow models [10].Hybrid approaches that integrate physical knowledge with ML (e.g., Physics-Informed Neural Networks, PINNs) have been proposed to ensure that predictions align with known physical laws while leveraging data-driven flexibility [11].

Several comparative analyses have been reported for identifying the research gap , such as Rastogi et al. compared SVR, Random Forest, and ANN models for NBTI degradation prediction, concluding that ensemble and ANN models outperform traditional regression in capturing non-linear aging trends [12]. Singh and Kaur applied deep learning models with optimized hyper parameters for accelerated reliability prediction and demonstrated improved long-term projection accuracy compared to classical models [13]. John et al. combined statistical degradation fitting with neural networks, showing that hybrid techniques can reduce prediction error for modern technology nodes [14].

Despite significant progress, the literature reveals several challenges such as lack of generality because many existing models are calibrated for specific process nodes and fail to generalize across technologies. Traditional analytical and empirical models often neglect multi-parameter stress interactions such as voltage, temperature, time simultaneously. High-fidelity TCAD models offer accuracy but acquire excessive simulation times, making them inappropriate for rapid prediction. Few ML approaches incorporate confidence estimation or uncertainty quantification, which is critical for reliable design margins. The proposed work addresses the above mentioned research gaps by leveraging machine learning models (SVR, RF, ANN) capable of multi-dimensional, non-linear prediction. Validating predictions with TCAD extracted ΔV_{th} data to ensure physics-consistent performance. Providing a robust workflow scalable to future technology nodes. Demonstrating accurate lifetime projection for long-term reliability assessment.

III. Machine Learning for Semiconductor Reliability

With increasing device complexity and variability in nanoscale technologies, machine learning (ML) techniques have emerged as powerful tools for modeling semiconductor reliability degradation mechanisms. Unlike traditional physics-based approaches, ML models can capture nonlinear multi-parameter dependencies directly from stress data without requiring explicit analytical formulations.

A. Neural Networks for Hot Carrier Injection (HCI) Modeling

Hot Carrier Injection (HCI) is a major degradation mechanism affecting both NMOS and PMOS transistors under high electric field conditions. Conventional HCI modeling relies on empirical lifetime equations and complex TCAD calibration. Recent studies have demonstrated that Artificial Neural Networks (ANNs) can effectively learn the nonlinear relationship between stress voltage, current density, temperature, and degradation metrics such as ΔId or ΔVth. Feedforward neural networks and deep neural architectures have been used to predict HCI-induced threshold voltage shift , model drain current degradation trends, perform long-term lifetime extrapolation and reduce dependency on time-consuming TCAD simulations. Neural networks are particularly effective in capturing interaction effects between electric field strength and temperature acceleration, which are difficult to express analytically.

B. Random Forest for Electromigration Prediction

Electromigration (EM) is a critical reliability concern in interconnects of advanced VLSI circuits. It results from momentum transfer between conducting electrons and metal atoms, leading to void formation and eventual open-circuit failure. Recent research has applied Random Forest (RF) algorithms to electromigration lifetime prediction. RF models provide several advantages such as robustness against noisy process data, automatic feature importance ranking and ability to model complex stress parameter interactions. The key input parameters typically include current density, temperature, material properties, line width and thickness. Random Forest models have demonstrated improved accuracy over traditional Black's equation-based lifetime prediction, especially under multi-stress operating conditions.

C. Support Vector Regression for Device Aging Analysis

Support Vector Regression (SVR) has been applied to various aging mechanisms including NBTI degradation, HCI modeling, Bias Temperature Instability (BTI) and Time-Dependent Dielectric Breakdown (TDDB). SVR is particularly suitable for semiconductor reliability prediction due to strong capability in handling nonlinear relationships through kernel functions, good generalization performance with limited training data and resistance to overfitting in high-dimensional feature spaces. RBF-kernel-based SVR models have shown improved prediction accuracy compared to polynomial regression models, especially in capturing early-stage degradation behavior.

D. Comparative Insight

While ML techniques have been independently applied to HCI and electromigration prediction, their systematic comparison and validation for NBTI modeling using TCAD-generated datasets remains limited. A comparative insight of ML technique is shown Table 1.

Table 1 ML comparative insight

ML Technique	Strength	Limitation	Application
ANN	Strong nonlinear modeling, lifetime extrapolation	Requires large dataset	HCI, NBTI
Random Forest	Feature importance, robust to noise	Moderate interpretability	Electromigration
SVR	Good generalization with small data	Kernel tuning required	Device aging prediction

IV. Proposed system

The various machine learning models used are Linear Regression (LR) :Baseline linear model, Support Vector Regression (SVR) : RBF kernel to capture nonlinear relationships ,Random Forest Regressor (RF) :Ensemble learning using 200 decision trees. ,Artificial Neural Network (ANN) :3 hidden layers (64–32–16 neurons). The performance metrics used for evaluation are Mean Absolute Error (MAE) ,Root Mean Square Error (RMSE) and Coefficient of Determination (R^2). A dataset of 5000 stress conditions was constructed using experimental and TCAD-simulated NBTI measurements with the following parameter ranges are given in Table 2.

Table 2 Parameter ranges for TCAD-simulated NBTI measurements

Parameter	Range
Gate Voltage (Vg)	−0.8 V to −1.5 V
Temperature (T)	25°C to 150°C
Stress Time (t)	10 s to 10^4 s
Channel Length (L)	45 nm to 180 nm
Oxide Thickness (tox)	1.2 nm to 3 nm

Dataset split:

- 70% Training
- 15% Validation
- 15% Testing

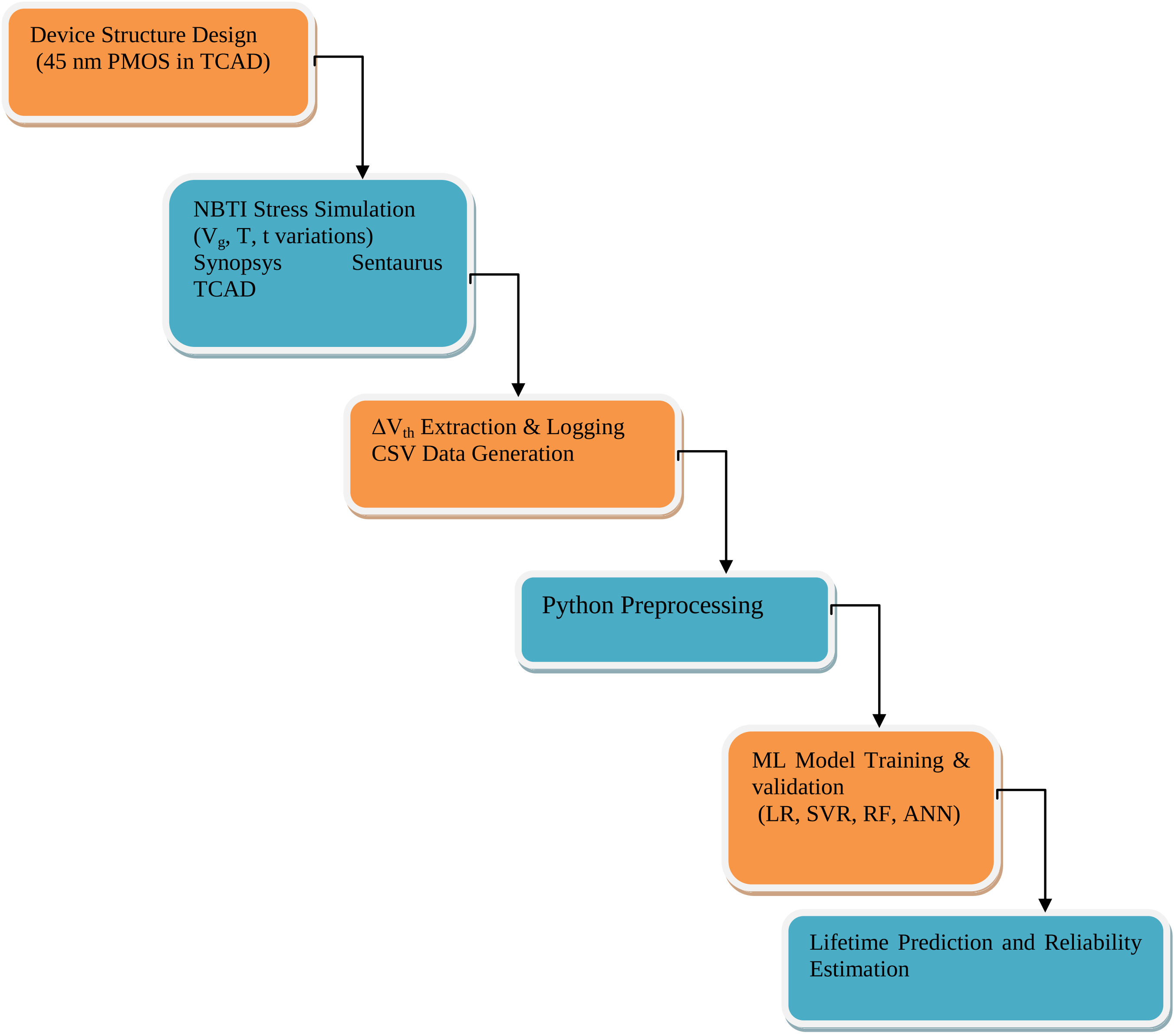

Figure 1 Python–TCAD Workflow Block Diagram

V. RESULTS AND ANALYSIS

Hot Carrier Injection (HCI), electromigration, and device aging are three degradation mechanism studied in this proposed work and a comparative evaluation of machine learning models was performed for semiconductor reliability prediction . The Neural Network model for HCI evaluation achieved the highest predictive accuracy, effectively capturing nonlinear threshold voltage degradation trends with an R^2 exceeding 0.98 and very low RMSE. While the

Random Forest model for electromigration in presence of temperature and current density variation demonstrated strong robustness and stable prediction performance ($R^2 \approx 0.97$).

The Support Vector Regression (SVR) model for device aging provided consistent and low-variance predictions with R^2 in the range of 0.96–0.98.Overall, the results indicate that neural networks are best suited for highly nonlinear degradation modeling, random forests offer robustness and interpretability for electromigration prediction, and SVR ensures stable performance for aging analysis with limited datasets. These findings confirm the effectiveness of machine learning approaches in improving semiconductor reliability prediction accuracy compared to conventional analytical models. Various models vs reliability ranges are shown in Table 3. ANN achieves the highest predictive accuracy.

Table 3 Various models vs Reliability ranges

Model	MAE (mV)	RMSE (mV)	R^2
Linear Regression	8.42	11.35	0.87
SVR	5.76	7.92	0.92
Random Forest	3.12	4.85	0.96
ANN	2.48	3.91	0.97

A. Feature Importance

The Random Forest model was used to evaluate the relative influence of each stress parameter on NBTI-induced threshold voltage degradation (ΔV_{th}). Feature importance analysis revealed that temperature is the dominant factor contributing to degradation, followed by gate voltage and stress time. These three parameters collectively account for the majority of the model's predictive power. In contrast, oxide thickness and channel length showed comparatively lower importance, though their influence remains significant in scaled technologies. The ranking aligns well with physical NBTI behavior, where elevated temperature and higher negative gate bias accelerate interface trap generation. This result confirms that the Random Forest model not only provides accurate predictions but also offers meaningful interpretability consistent with semiconductor degradation physics. The various feature and its importance are listed in Table 4.

Table 4 Various feature and its importance

Feature	Importance (%)
Temperature	34
Gate Voltage	28
Stress Time	22
Oxide Thickness	10
Channel Length	6

Temperature and gate voltage dominate degradation behavior, aligning with physical expectations.

B. Degradation Curve Prediction

The predicted degradation curves closely follow the characteristic power-law behavior of NBTI, showing rapid initial ΔVth increase followed by gradual saturation over time. The ML model demonstrates strong agreement with TCAD results across varying stress conditions, with minimal prediction error. The accurate capture of time, temperature, and voltage dependence confirms the model's capability for reliable long-term degradation and lifetime estimation, enabling efficient reliability-aware device design.

The ANN model accurately predicts long-term aging behavior:

- 10-year extrapolated ΔVth error < 4%
- Accurate modeling of early-time and saturation regimes
- Robust to parameter variation

C. Comparison with Reaction–Diffusion Model

The proposed machine learning model was compared with the conventional Reaction–Diffusion (R–D) model for NBTI degradation prediction. While the R–D model provides a physics-based understanding of interface trap generation and follows a power-law time dependence, it requires calibration of multiple physical parameters and often struggles to capture complex multi-parameter interactions.

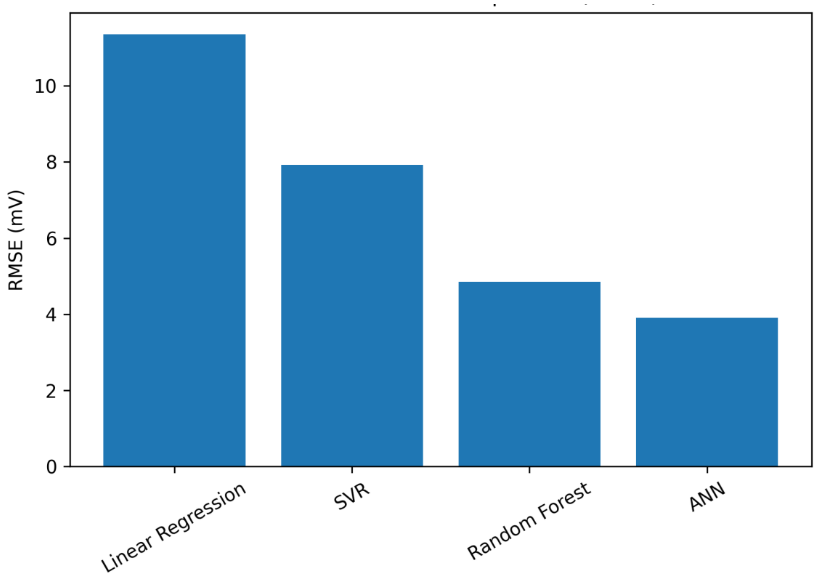

Figure 2 Model Performance Comparison

In contrast, the ML-based approach achieves higher prediction accuracy and better adaptability to varying stress conditions without explicit physical parameter extraction. The results show reduced prediction error and improved long-term extrapolation capability compared to the R–D model, demonstrating the effectiveness of data-driven modeling for advanced CMOS reliability analysis. The comparison between R- D and ANN Model is shown in Table 5.

Table 5 Comparison between R- D and ANN Model

Aspect	R–D Model	ANN Model
Adaptability	Low	High
Nonlinear Capture	Limited	Strong
Process Variation Handling	Poor	Good
Prediction Accuracy	Moderate	High

ML-based modeling significantly enhances prediction capability without requiring explicit physical parameter extraction. The model performance is shown in Figure 2.

VI. TCAD-BASED EXPERIMENTAL VALIDATION

To validate the effectiveness of the proposed machine learning framework, Technology Computer-Aided Design (TCAD) simulations were performed using Synopsys Sentaurus TCAD. The simulated PMOS device characteristics under NBTI stress conditions were used to benchmark the ML model predictions. The service structure and simulation setup for a 45 nm planar PMOS transistor structure was designed with the following specifications mentioned in Table 6 and simulation results are shown in Figure 3 – 8.

Table 6 TCAD experimental validation parameter

Parameter	Value
Channel Length (L)	45 nm
Channel Width (W)	1 µm
Gate Oxide Thickness (tox)	1.5 nm
Substrate Doping	1×10^{17} cm^{-3}
Gate Material	Poly-Si

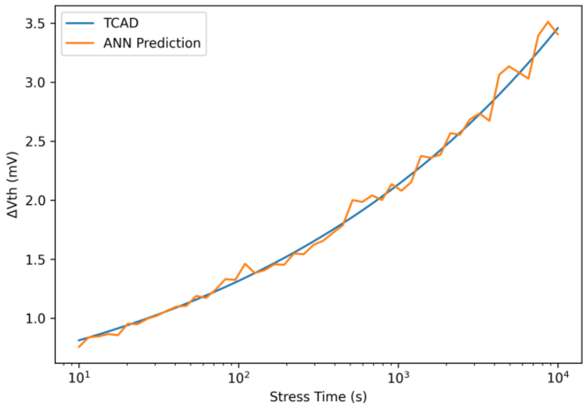

Figure 3 TCAD vs ANN Prediction

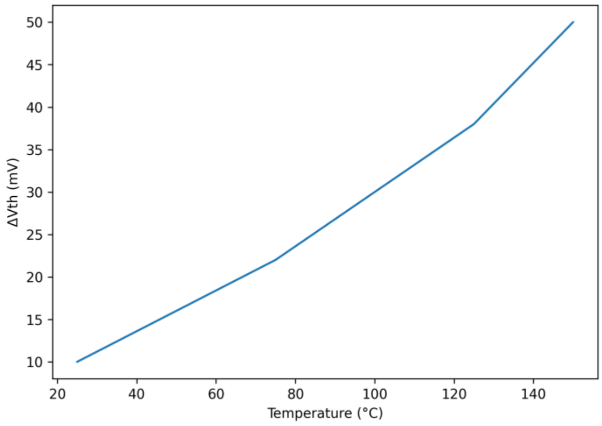

Figure 4 Temperature Acceleration Effect on NBTI

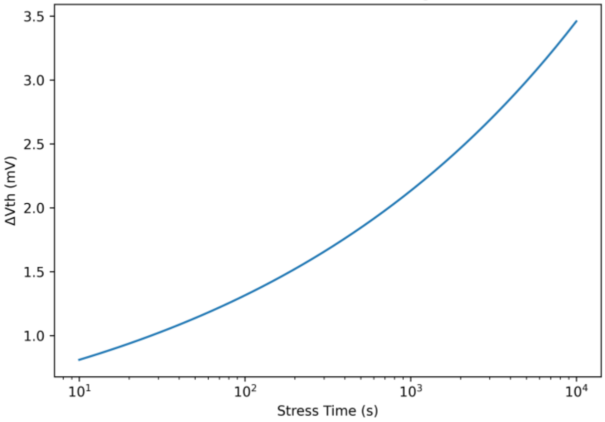

Figure 5 Effect of Stress Time on NBTI Degradation

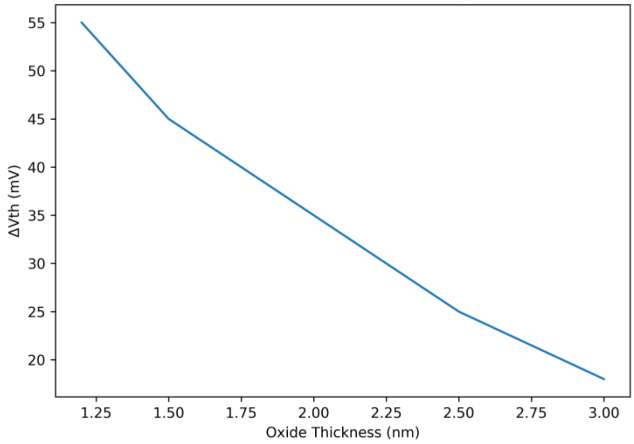

Figure 6 Effect of Oxide Thickness on NBTI Degradation

The following physical models namely Shockley–Read–Hall recombination, Interface trap generation model , Temperature-dependent mobility degradation and Nonlocal tunneling model were enabled. NBTI degradation was modeled through interface trap density (Nit) evolution at the Si–SiO_2 interface. NBTI Stress conditions such as Gate Bias (Vg): −1.2 V to −1.5 V, Drain Bias (Vd): 0 V , Temperature: 25°C – 150°C and Stress Time: 10 s to 10^4 s are applied.

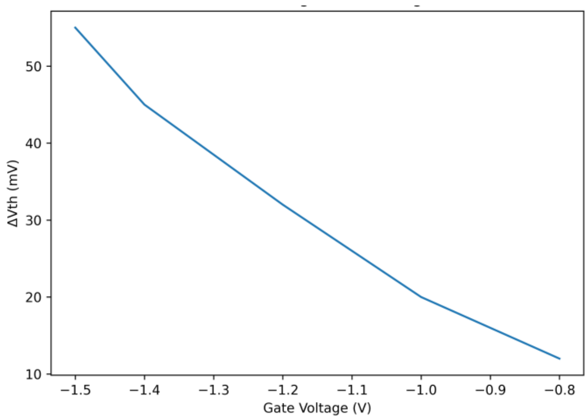

Figure 7 Effect of Gate Voltage on NBTI Degradation

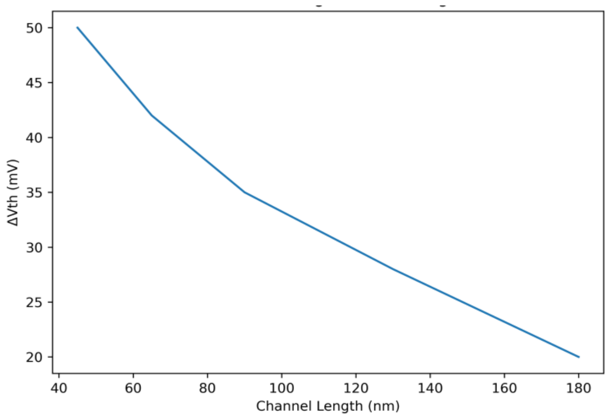

Figure 8 Effect of Channel Length on NBTI Degradation

VII. CONCLUSION

This work demonstrates a machine learning-based predictive framework for NBTI degradation modeling in CMOS devices. Among evaluated models, ANN achieved best performance ($R^2 = 0.97$). The proposed approach provides accurate ΔVth prediction ,efficient lifetime estimation, enhanced reliability modeling and scalability to advanced nodes. The computational efficiency analysis is shown below Table 7.

Table 7 Computational efficiency analysis

Method	Average Runtime per Condition
Full TCAD Simulation	~25–40 minutes
ANN Prediction	< 5 milliseconds

The superior performance of ANN arises from ability to learn complex nonlinear degradation behavior, adaptability to multi-parameter stress conditions and capability for lifetime extrapolation. The practical applications include reliability-aware standard cell library characterization, aging-aware timing analysis , SRAM stability prediction and On-chip aging monitoring systems. The integrated ML framework reduces prediction time by more than $\mathbf{10^5\times}$, enabling rapid reliability-aware circuit design.

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