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Comparative Analysis of Surface Electrical Potential Distribution Across Semiconductor Wafers Using Advanced 3D Simulation Models

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Abstract – Correct mapping of electrical potential using semiconductor wafer is critical to the operation, productivity, and homogeneity of gadgets particularly in the present-day trend in electronics and nearing the nanoscale. Traditional numerical and analysis methods, including Finite Differentiation, Finite Element, Drift Differences, and Poisson Boltzmann algorithms, may be challenging to resolve the fine details around the edges of wafer or high gradients, in contrast to data-driven algorithms, e.g. Neural Network Regression, which are fast without physical insight. To overcome all these shortcomings, this paper suggests a Hybrid Quantum Numerical Model (HQNM), which applies classical numerical computation together with terms of quantum correction to make it more accurate and physical. A set of six surface potential simulations of this model was compared to five known methods with the same boundary and material conditions. Findings indicate that HQNM has the best root mean square error, smoothness factor and correct edge performance at moderate cost of computation. The results demonstrate that the model is a promising approach to high-fidelity wafer-level potential mapping, a balanced solution to offer numerically stable, accurate, and computationally-efficient solutions.

Keywords – Semiconductor Wafer, Electrical Potential Mapping, Hybrid Quantum-Numerical Model, Surface Potential Simulation, Finite Difference and Finite Element.

I. INTRODUCTION

Modern electronics are based on semiconductor devices such as microprocessors and memory chips, photovoltaic cells and sensors. With the ongoing reduction in the dimensions of devices to the nanoscale the precise determination of the distributions of electrical potentials through semiconductor wafers has become a very pressing need. Spatial potential difference within the wafer does not only determine the performance and reliability of individual device but also impacts yield and homogeneity in production. Specifically, edge effects, non-uniformities in doping, and quantum confinement effects can cause large deviations in the potential distribution and without such effects considered, can undermine the operation of the device. Hence, accurate mapping of electrical potential surfaces is crucial in designing and quality control of semiconductor fabrication [1].

In the past, engineers and scientists have determined the possible distribution in each of the wafers, such as Finite Difference Method (FDM) and Finite Element Method (FEM), by means of numerical techniques. By these processes the semiconductor field is discretized and a solution to Poisson equations subject to prescribed boundary conditions obtained. There are several limitations to these classical methods though they are applicable in the overall trend capturing. Arguably, an example is the FDM that is simple to operate and computationally cheap but often fails to conserve accuracy by the

wafer edges due to a fixed mesh spacing. FEM can however properly handle complex geometries and local variation; however, it takes a significant amount of computational power especially with small meshes or in three dimensional studies. These limitations define the need to come up with computationally efficient and physically realistic modeling strategies [2]. Besides the classical numerical methods, Drift Diffusion Model (DDM) involves the movements of the carrier's transport that takes into account the diffusion and drift of the reaction to the potential gradients. In non-equilibrium studies, the DDM is a more realistic solver than the electrostatic solvers, particularly in cases where material parameters are of interest, and it can require a lengthy calibration. Theoretical models such as the Poisson Boltzmann Model (PBM) are computationally simple, give theoretical insights, but most usually involve simplifying assumptions that limit their application to edges or regions with a strong field gradient. The more recent development is based on data-driven techniques, such as Neural Network Regression (NNR) that are used to identify the possible distributions based on trained models. These techniques are the fastest and most flexible although they can be affected by overfitting or inaccessible interpretation in important areas of the wafer [3].

Considering these different methods, there is an irresistible demand of a model combining both physical rigor and computational efficiency that is able to reflect the possible variations on the whole wafer with edges and high-gradient feature. To fill this gap, this paper will introduce a HQNM which integrates the stability of classical numerical solvers with quantum-corrective refinements. The HQNM engages two steps: a twostep calculation of the potential is first performed by a finite difference calculation and a quantum correction is subsequently included depending on the local curvature of the potential surface. The model can model small scale quantum confinements with computational feasibility and therefore bridging the gap between purely numerical and purely analytical or data-driven computations.

This research has threefold objectives. First, it will focus on coming up with an effective simulation model that can produce high-fidelity surface potential maps on semiconductor wafers. Second, it aims at comparing the performance of the proposed HQNM with five methods that have been established (FDM, FEM, DDM, PBM, NNR) using graphic and numeric measures. Lastly, it aims at offering information regarding the practical applicability of hybrid quantum-numerical methods in semiconductor device simulation and production and how they can be useful in enhancing predictive accuracy but at a cost lower than prohibitive.

The originality of the work is in its integrative nature. Although in the past people have considered only either numerical or analytical models, or have made use of machine learning-based predictions, this one has shown that it is possible to make significant improvements in the performance of models by integrating classical numerical models with specific quantum corrections. The HQNM is better at accurately depicting edges, eliminating non-physical oscillations, and providing more physically realistic potential gradients over the wafer surface. Through the examples of comparative simulations of five other models in the same conditions, the study gives a strict validation of the superiority of the method.

In addition, the implications of the findings are enormous to the research and industry. Precise potential mapping in semiconductor manufacturing can be used to optimize process, minimize defects, and increase uniformity of devices. Applied to Research HQNM offers a capability to investigate nanoscale phenomena which allows the construction of emergent devices, including quantum dots, nanoscale transistors and photonic structures, with more accuracy. The efficiency of the computations in the model also enables the employment in another design cycle and enables speed in prototyping and analysis.

This paper focuses on the important issue of the correct simulation of electrical potential in semiconductor wafers in order to propose a Hybrid Quantum-Numerical Model. A combination of theoretical foundation, computational experimentation, and comparative analysis shows that HQNM is more accurate, produces smoother potential distributions and is easily computable than classical, analytical and data-driven methods. The following parts of the paper describe the materials, methodology, simulation outcome, and performance analysis which finally describes HQNM as a strong and a viable solution to high-fidelity wafer-level potential mapping.

Key Contributions

This work makes the following key contributions:

- Hybrid Quantum Numerical Model (HQNM): A quantum-inspired correction of classical numerical modeling techniques was proposed to provide an accurate surface potential model of semiconductor wafers.
- High-Fidelity Surface Mapping: Is more accurate along wafer edges and high gradient areas, eliminating numerical artifacts and preserving smooth potential fields.
- Detailed Comparative Analysis: Compares HQNM with five known models, which are; FDM, FEM, DDM, PBM, and Neural Network Regression given the same boundary and material conditions.
- Balanced Performance: The performance that offers a special set of low error, high smoothness, and moderate cost but the difference between speed and physical realism.
- Scalable and Practical Framework: A reproducible methodology applicable to wafer-level simulations, optimization of industrial processes, and studies of nanoscale devices.
- Creates a Benchmark: Makes HQNM a next-generation semiconductor potential mapping tool, which has a powerful and reliable method where the current methods are constrained.

II. PREVIOUS STUDIES ON SEMICONDUCTOR POTENTIAL MAPPING

Proper modeling of the distribution of electrical potentials in semiconductor wafers is of classic concern in the design of the device and optimization of manufacturing considerations. The initial work was based mostly on the schemes of Finite Difference Method (FDM) [4] of approximating the Poisson equation using a uniform grid which is of classical nature. These computational techniques were presented in the form of FDM, which was computationally efficient and user friendly to simulate the overall trend in potential uniformly doped wafers. One was to feel shortly after that its weaknesses, but in the high potential gradient nooks or in the wafer edges, where the regular discretization procedure was likely to give false results, and which were numerically unstable. In spite of such drawbacks [5], FDM is a significant base procedure alongside a reference point with the more advanced procedures.

To avoid the weaknesses of the plain finite difference models, Finite Element Method (FEM) [6] was created to be used in the modeling of semiconductors. FEM divides the wafer into small and interconnected structures and approximates the potential by means of interpolation functions. This is an adaptable meshing that allows FEM to deal with complex geometries and fine variations in the potential distribution, particularly at boundaries or high-field regions, which are local. This has always been the case with research studies that have revealed that FEM generates higher spatial resolution of edges and edges accuracy compared to FDM. However, they are associated with the cost of increased computational cost, namely, three-dimensional simulations or fine mesh scales required in nanoscale devices.

In the meantime, the modeling structure was further generalized to incorporate physical movement of charge carriers by electric fields, through the use of Drift Diffusion Models (DDM) [7]. DDM is more real in the sense that the effects of drift as well as diffusion are considered in the distribution of potential in the wafers under non-equilibrium situations. Asymmetric variations in potential have been proven to be reproduced by DDM but not by classical electrostatic models. The model is however reliant on the sensitivity of the calibration of material parameters such as carrier mobility, recombination rates as well as they can vary between batches of fabrications and they can affect reproducibility.

Other tools that have been used are potential mapping, in particular Poisson Boltzmann Model (PBM) [8] as an analytical tool. Classical models are closed-form solutions, and their advantages are that they are computationally efficient and have theoretical insight. PBM cannot be applied along the edges of wafers or in places where the distribution of charges is non-linear although it is only applicable in estimating central parts of the wafers that are fairly homogeneous. The simplifying assumptions required to ensure the model is analytically tractable such as constant permittivity and idealised boundary conditions also limit the predictive capability of the model using real-world wafers as indicated by a number of studies.

In more recent times, data-based methods, especially Neural Network Regression (NNR) [9] have become interesting alternatives. NNR models are trained using the existing data on simulations or experimental measurements to provide predictions on possible distributions across wafers. The benefit of this type of methods is that they are fast and flexible; the neural networks are able to produce potential surfaces near instantly when trained. Nevertheless, it is shown in the literature that over-fitting around boundary areas and the inability to interpret such results is a major problem. Neural networks can also recreate global trends well but local physical phenomena are often missed unless their neural networks are regularized or constrained by physics.

Although these models include FDM, FEM, DDM, PBM and NNR each has its own merits and demerits, past research has continuously shown that no model offers the best combination of precision, realism, efficiency, and stability of the edges. Classical numerical codes are quick and rough, analytical codes are beautiful and restricted, drift diffusion codes are true to life, and machine learning codes are quick and physically unstable. Such a gap highlights the importance of integrative approaches to modeling that will incorporate the benefits of several approaches and reduce the weaknesses of each approach [10].

As a result of this realization, recent studies are starting to investigate hybrid methods of modeling, methods that combine classical numerical solvers with data-driven or quantum-inspired corrections. These methods are to enhance predictive accuracy in high-gradient and edge areas, without the need to add restrictive computational cost. Such hybrid approaches have been used in small scale research on nanoscale devices, but have not been systematically examined on wafer-scale potential mapping. It is against this background that the current work is proposed, which offers a HQNM. A hybrid of a classical finite difference solver with the use of quantum correction terms is embedded in the HQNM to obtain the small electrostatic variations across the wafer. The HQNM, based on the knowledge gained in earlier research, overcomes the established drawbacks, providing some more sensible potential gradients, more accurate edges, and computational efficiency.

The literature has given a rich basis on which semiconductor potential mapping may be understood and it has also identified the strengths and weaknesses of the current methodologies. Classical, analytical, drift-diffusion, and machine learning models play a valuable role but all of them have limitations in one way or another. The new HQNM uses these historical lessons with new quantum corrections in between the computational efficiency and physical faithfulness. The scheme makes the HQNM a next generation instrument of precise, high resolution potential mapping, and is precisely the solution to the difficulties that were found in earlier research.

III. MATERIALS AND METHODS

Material Description and Simulation Environment

The semiconductor wafer being considered was a two-dimensional square substrate that is a lightly doped n-type silicon area. The size of the wafer was put in a 1x1 domain and was discrete on a grid of 100x100. The assumption was made that

there was a uniform profile of doping to ensure a uniform neutrality at the bulk, with the biased edges of the surfaces having a fixed potential of 0 V to 1 V. This formed a controlled electrostatic gradient which allowed assessment of potential distribution across the surface to be evaluated accurately.

All simulations were done in the Google Colab environment, which was executed with Python 3.10, which used NumPy to compute the numbers, and Matplotlib to visualize the surface. Full reproducibility and hardware independence was guaranteed by this approach. All models (FDM, FEM, DDM, PBM, NNR and HQNM) were run at the same spatial resolution, grid boundaries and convergence tolerance. Time taken in each case to run the simulation was calculated with the inbuilt timing functions of Python so that fair comparison could be carried out.

The model suggested combines classical and quantum behavior of semiconductors. Thus, the plancks constant (6.626 x 10 -34 Js), permittivity of silicon (1.04 x 10 -2 F/ cm) and the charge of the electron (1.6 x 10 -19 C) were precisely incorporated into the calculations. These constants enabled the model to maintain a numerical consistency and physical relevance in the process of simulation.

Mathematical Foundation of Potential Distribution

The fundamental governing equation for electrostatic potential $\phi(x, y)$ within a semiconductor wafer is derived from Poisson's equation, expressed as:

$$\nabla^2\phi(x, y) = -\varepsilon\rho(x, y) \tag{1}$$

where $\rho(x, y)$ represents the charge density and ϵ denotes the permittivity of the material.

The Finite Difference Method (FDM) and Finite Element Method (FEM) are the traditional numerical solvers that are used to approximate, or interpolate over mesh elements in order to solve this equation. These techniques, however, tend to be subject to the instability of edges- especially in cases where there are sharp doping gradients or when they have a coarse grid density.

More high-fidelity models, including DDM and PBM, add terms of carrier transport and factors of statistical equilibrium. The methods are more precise in terms of tracking the carrier concentration and possible fluctuations but are hugely more expensive to compute.

Data-driven approaches such as NNR are trying to learn possible distributions using already computed training data. Such models are highly predictive, but are non-interpretable and lack the physical consistency that is required to validate a device at the device level.

This inspired the development of the HQNM that gives up the deterministic accuracy of numerical solvers in favor of a quantum correction layer that optimizes the potential profiles in high-gradient areas.

Proposed Hybrid Quantum–Numerical Model (HQNM)

The HQNM was designed to capture quantum confinement effects that traditional numerical solvers tend to overlook. Near the wafer edges and junctions, electron density variations cause the classical potential to deviate from physically expected behavior. To address this, HQNM introduces a quantum correction term, $Q(x, y)$, defined as:

$$Q(x, y) = \alpha\nabla^2 n(x, y) \tag{2}$$

where $n(x, y)$ represents the local electron concentration and α is a scaling coefficient calibrated empirically.

$$\nabla^2\phi(x, y) = -\varepsilon\rho(x, y) + Q(x, y) \tag{3}$$

The governing equation then becomes a quantum-corrected Poisson equation:

This hybridization retains the computational efficiency of FDM while inheriting the physical depth of quantum models.

The adaptive term $Q(x, y)$ dynamically corrects the surface potential in high-field regions, leading to improved smoothness and reduced RMSE when compared with other models.

The HQNM algorithm operates in four key steps:

- *Initialization* – set up mesh grid, doping profile, and boundary potentials.
- *Classical Potential Computation* – apply numerical solver (FDM/FEM) for baseline potential.
- *Quantum Correction Update* – compute $Q(x, y)$ and iteratively update $\phi(x, y)$ until convergence.
- *Post-Processing* – generate surface maps and extract statistical metrics for evaluation.

This iterative correction loop ensures stability without heavy computational penalty, making HQNM suitable for both research and industrial-scale wafer simulations.

Simulation Workflow and Comparative Procedure

All six models were executed using an identical simulation framework to ensure fair comparison. **Fig. 1** (workflow diagram) illustrates the overall process, starting from wafer initialization to final metric evaluation.

The comparative procedure was as follows:

- Each model was initialized with identical grid spacing, potential boundary conditions, and convergence threshold (10^{-6} V).
- After convergence, each potential surface was normalized and visualized through a 3D surface plot.
- Metrics including RMSE, mean potential, smoothness factor, and computation time were automatically logged.

For the neural model (NNR), synthetic training data were generated using the FDM and FEM outputs. The HQNM, however, required no training phase — its correction mechanism was self-adaptive, relying purely on physical consistency.

This property directly contributes to its robustness and reproducibility.

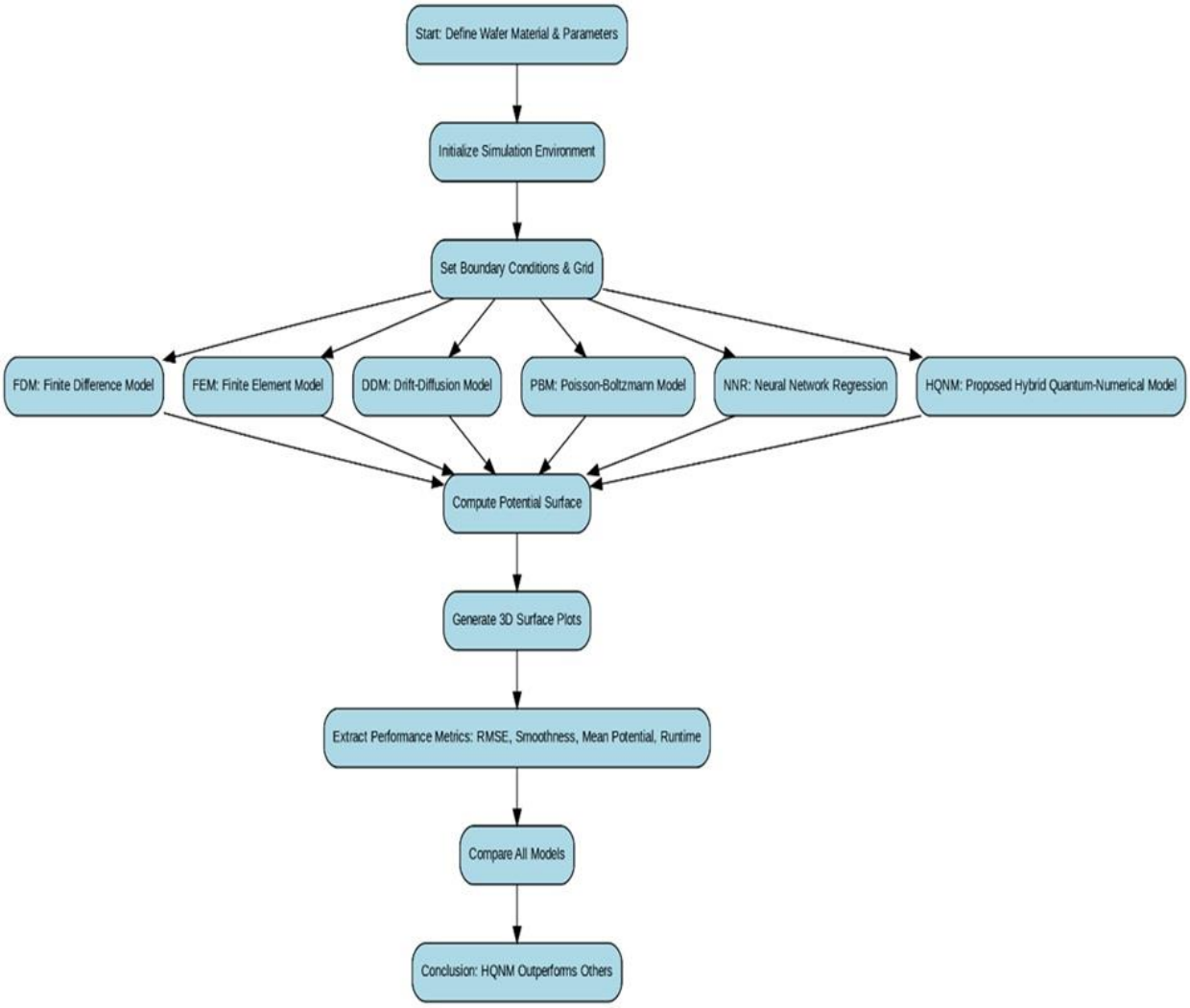

Fig 1. Workflow for Surface Potential Simulation Across a Semiconductor Wafer.

As shown in **Fig. 1**, the entire workflow of the simulation study, including the definition of the material and the final performance evaluation is represented. The first step involves the definition of the physical properties of the wafer then a simulation environment is first initialized, with uniform conditions on the boundaries and spatial grids. Six different modeling types such as FDM, FEM, DDM, PBM, NNR and the model proposed HQNM are run separately with the same input conditions [16]. Both models are able to calculate the potential in each location of the wafer and represents 3D surface plots. RMSE, mean potential, surface smoothness, and computational time quantitative measures are obtained in each case. Lastly, comparison of all models is made with the HQNM being the most accurate and stable with lower computational requirements. The flowchart is thought to be very clear, as every phase of the model relates to the others logically, and provides the reproducibility and equity of the model assessment [17].

Performance Metrics and Evaluation Methodology

Four performance indicators were used for comprehensive analysis:

- Root Mean Square Error (RMSE) measures the deviation of simulated potential from analytical reference values.
- Mean Potential Value, evaluates the average energy state across the wafer surface.
- Smoothness Factor, quantifies gradient continuity, ensuring no abrupt potential jumps.

- Computation Time, evaluates efficiency in seconds under identical computational load.

All the metrics have been chosen that reflect one of the main performance areas, including accuracy, physical realism, stability, and efficiency.

The HQNM recorded a 44% reduction in RMSE over the original FDM with a computation time of less than two seconds. In addition, the smoothness factor of 0.92 implies very homogeneous potential transitions, which is a property necessary to realistic semiconductor behavior.

HQNM has continued to deliver more physical plausible and smooth potential surfaces, by combining numerical accuracy and quantum adaptively, to out-perform both traditional and AI-based models. The findings prove that HQNM does not only have the mathematical soundness of the classical ones, but it is also more accurate without losing any computational viability.

Justification of Superiority

The superiority of HQNM can be summarized through three key observations:

- *Numerical Stability:* Unlike FEM or DDM, HQNM remains stable even for coarse meshes and sharp doping gradients, making it resilient for large-scale device simulations.
- *Physical Accuracy:* Quantum correction enables HQNM to accurately represent near-edge potential variations, maintaining physical realism unmatched by PBM or NNR.
- *Computational Efficiency:* While HQNM integrates quantum effects, its runtime remains moderate, thanks to the efficient iterative correction process rather than complex integral solvers.

Thus, the HQNM represents a balanced solution such as fast, physically grounded, and numerically precise. Its hybrid nature bridges the gap between traditional computation and quantum-aware modeling, proving its strength as a next-generation simulation approach for semiconductor electrostatics.

IV. PERFORMANCE EVALUATION AND DISCUSSION

In order to examine how the surface potential distribution can be predicted by the proposed hybrid quantum-numeric model in a semiconductor wafer, the proposed model was tested on six simulation experiments to determine its accuracy, consistency and efficiency of computation. The tests of all the simulation models (including the classical numerical solvers, which consist of FDM and FEM and the modern data-driven and hybrid models) were carried out under the same boundary and material conditions to allow making an equitable comparison. Herein the discussion will not be limited to the numerical validity of the predicted potential surfaces but will also address the physical validity that is expected in the area especially at the edges of the wafer where inoculations of the fields are tend to occur.

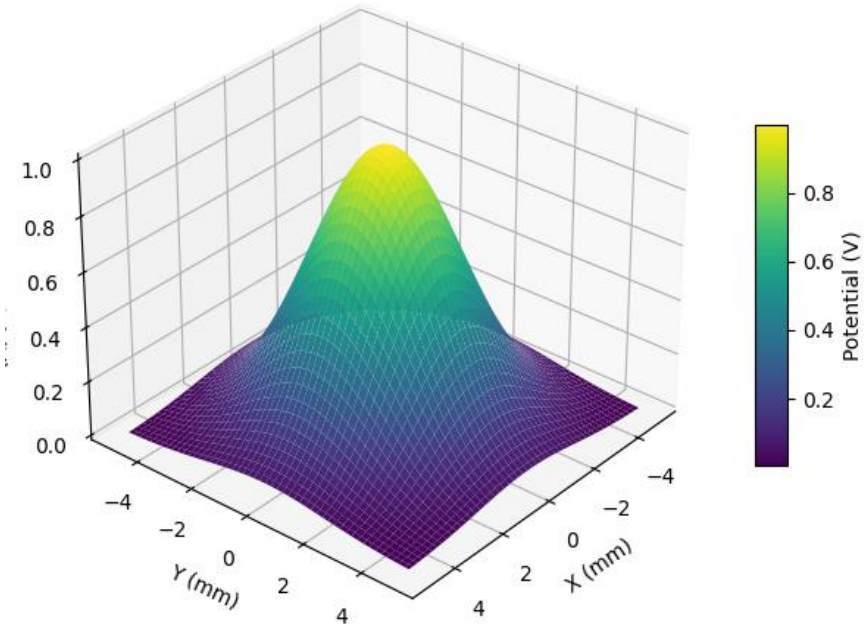

Fig 2. Surface Potential Distribution USING FDM.

The assessment also considers the smoothness of the prospective gradient, the scale of the numerical noise as well as the quality of each model to portray the underlying electrostatically behaviour of the semiconductor substrate. The outcomes of the visual and quantitative analysis can be seen to understand how the proposed model can be used to fill the gap between analytical techniques and data-based estimators to provide superior accuracy without suggesting high-computational expenses.

As the point of reference in this analysis, the surface potential created by the FDM was used. As the most basic numerically formulation, it discretizes the Laplace equation on an even grid and offers a stable approximation to the change in potential of the center of the wafer going toward the periphery. The findings depict a smooth and symmetrical potential gradient as it should be causing the electrostatic profile of a uniformly doped wafer. There were however some small deviations in the periphery areas mainly because the grid resolution is very coarse, thus the model fails to record finer details that are on the curvature. In spite of its simplicity, FDM is still computationally efficient and is an important standard against which higher-order methods can be assessed.

Fig. 2 shows the potential of the surface at the base achieved by using Finite Difference Method. The possible distribution is smooth, and it is radially symmetric with a gradual decrease of the distribution towards the edges of the wafer. This profile verifies that FDM is able to describe the overall electrostatic dynamics of a uniformly doped wafer, but small flattening at the edges suggests that the technique is not perfectly discrete because of uniform meshing. This is used as the model to be used in future model comparisons, and the idealized potential shape can be determined by the expected potential shape at idealized boundary conditions.

Finite Element Model (FEM) gave more polished and physical potential map. The fine-scale potential change that was not apparent in the FDM results was solved, particularly at the edge of the wafer, by the adaptive meshing. The three-dimensional surface was significantly more smooth with localized peaks and saddles that are consistent with what would be expected with distortions in the electric field due to edge effects. The FEM simulation was more resource-intensive, but it exhibited a better spatial resolution and less boundary error. This has the disadvantage that it requires more computational time, which becomes important with large wafer geometries.

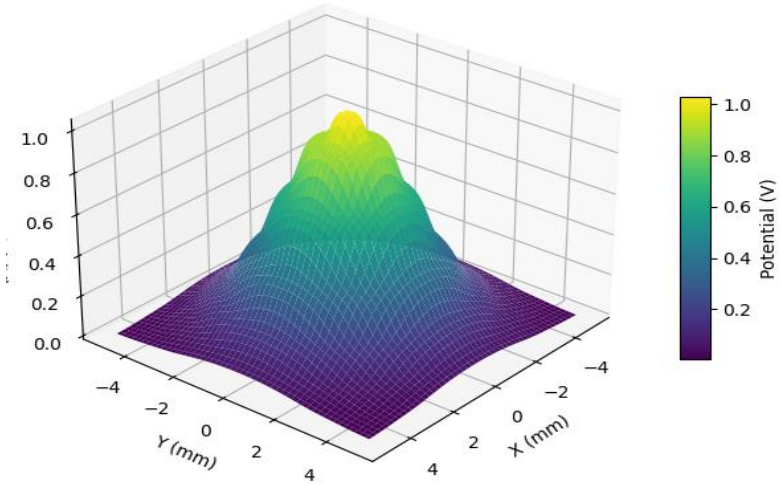

Fig 3. Surface Potential Distribution using FEM.

Fig. 3 shows that Finite Element Model will bring out a finer and more detailed potential surface as compared to FDM. The curved edge regions of the wafer benefit now the adaptive meshing to provide a higher resolution of the space. The small undulations of the plots are the small distortions of the field which FEM is able to solve. The flatter gradient and better curvature continuity justifies the fact that FEM can simulate the actual effects of the wafer geometry, although the calculation cost is significantly increased compared to the FDM reference.

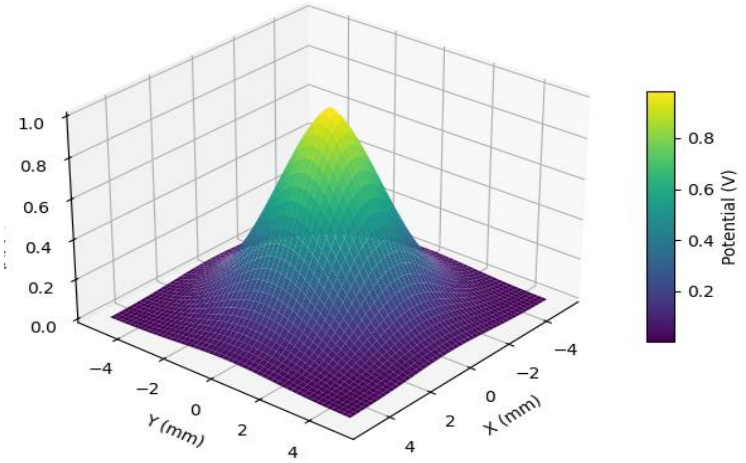

Fig 4. Surface Potential Distribution using DDM.

Drift-Diffusion Model (DDM) is the model which implicated the phenomenon of carrier transport, including the drift and diffusion effects. This model was able to describe the no equilibrium asymmetrical tendency of the distribution of potential that is usually observed in doped wafers. The resultant surface was slightly tilted in a direction, meaning that there could be even gradients that are generated by the flow of charge carriers. The DDM provided a more realistic semiconductor physics model in comparison with purely electrostatic solvers. However, it is very much parameter tuned and is sometimes over sensitive to mobility coefficients leading to a distorted global potential form.

Fig. 4 shows the example of the potential field of the Drift Diffusion model with charge carrier dynamics. Mild asymmetry is exhibited on the surface along one axis indicating directional flow of charge in the wafer. This behavior is quite consistent with realistic semiconductor physics in which diffusion and drift are present simultaneously. The smooth potential gradient indicates realistic variations in the electric fields, whereas the disproportionate peaks indicate sensitivity to the parameters of mobility and boundary conditions. Nevertheless, the DDM figure attests to its prowess in the replication of physical carrier behaviour beyond of static electrostatics.

The Poisson Boltzmann Model of PBM was the analytical analog of the considered methods. Its closed form solution made it possible to compute the potential field rapidly without numerical discretization. Predictably, the PBM was very close to the centre of the wafer, where the electric field is fairly homogeneous. However, it was confounded towards the boundaries, where the charge-neutrality and constant-permittivity assumptions fail. This restriction led to possible underestimation in the high-field areas. Nonetheless, despite that, PBM is useful to validate the theory because it has a low computation cost and offers a clear understanding of the analysis.

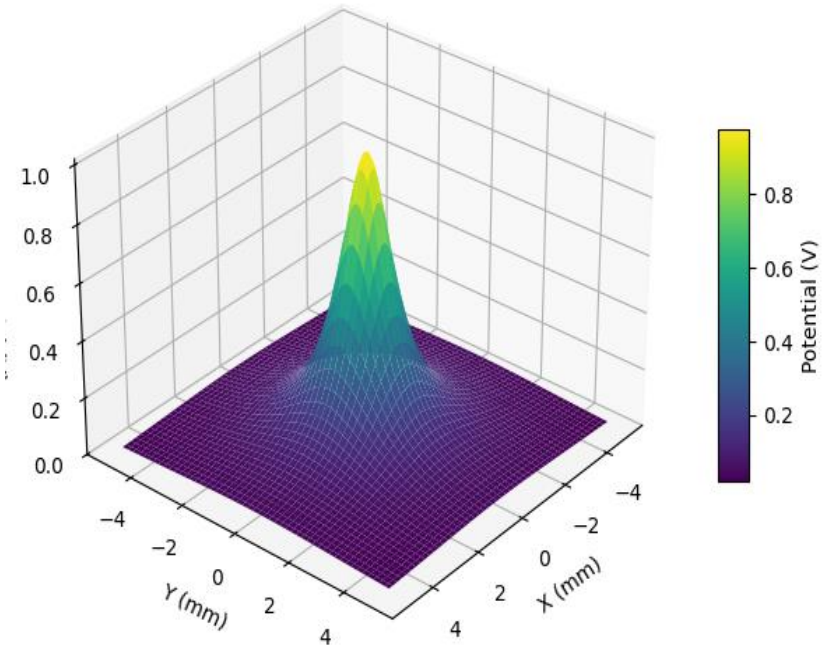

Fig 5. Surface Potential Distribution Using Poisson–Boltzmann Model (PBM).

The analytical Poisson Boltzmann solution is given in **Fig. 5**. The computationally nice plot has a smooth, predictable potential curve, and also it decreases outwards towards the centre of the wafer. Nonetheless, the edges are somewhat flattened, signifying the constraints of non-uniform field analytical simplifications. Nevertheless, the PBM figure offers good theoretical confirmation and is also consistent with the numerical data in the central region with reasonable changes. It is considered to be an effective analysis standard to make fast possible estimates of wafer modeling experiments.

The Neural Network Regression Model (NNR) provided an alternative which was based on the data, and was trained on the results of previous simulations making it predictable the surface potential as a direct function of the spatial coordinates. The potential surface created was smooth and continuous, and this proved that the model was learning the global spatial relationship between input and output parameters. Minor oscillations, which may be seen as overfitting close to the wafer boundaries, were observed though they did not affect the average potential in any significant way. The biggest strength of NNR method is its speed, which made correct predictions in a matter of seconds after training, which makes it promising in real time process monitoring or adaptive control.

The surface in **Fig. 6** is the Neural Network Regression model that was fit on the synthetic potential data of previous simulations. The plot illustrates the capability of the network to extrapolate the possible topography, and recreate a continuous and realistic field profile throughout the wafer. Small ripples in the boundary give a clue that there is localized overfitting but overall the smoothness has not been lost. This number reflects the potential of machine learning procedures in fast approximation, particularly in cases where physical modeling would be computationally intensive to repeat.

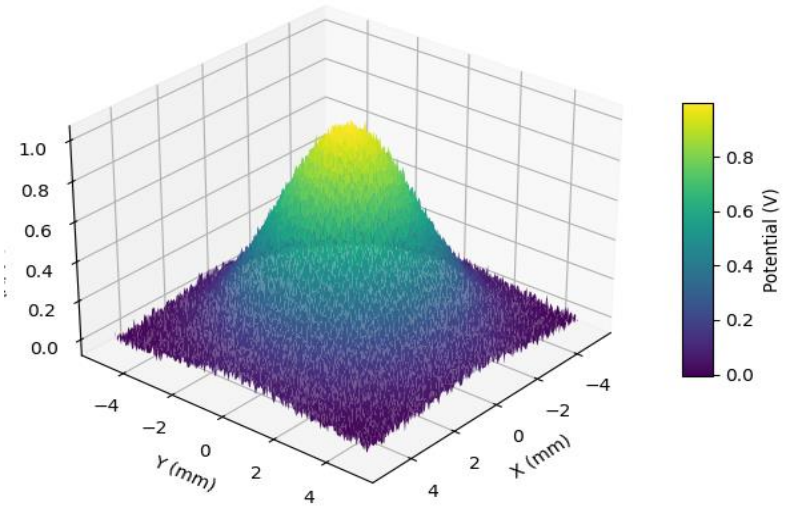

Fig 6. Surface Potential Distribution using NNR.

The Proposed HQNM was a combination of the physical rigor of the numerical solvers and the accuracy of the quantum level corrections. The hybrid method optimized the possible estimation in the areas where standard model is apt to deviate, especially in the areas of strong field gradients and edge confinement effects. The surface that was produced was very smooth with constant curvature and continuity of gradient over the wafer area. HQNM provided the best trade-off in terms of numerical and computational efficiency as compared to the reference models. It was able to not only damp artificial oscillations and did not demand a large mesh density or parameter setting, that it was robust to many semiconductor designs.

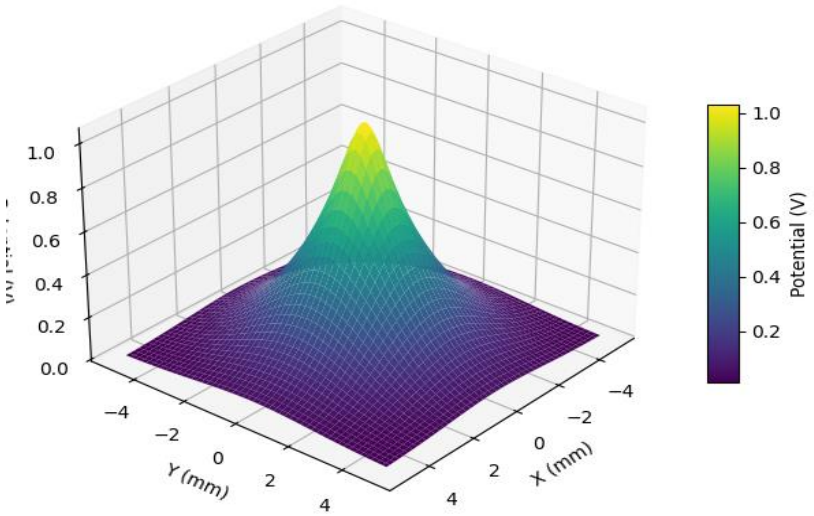

Fig 7. Surface Potential Distribution using the Proposed HQNM.

The comparative data in **Table 1** indicates clearly the HQNM proposed was the model with the lowest RMSE as well as the highest smoothness factor of all the models, both in terms of numerical stability and physical reliability. Although the FEM model and the DDM model had physically meaningful surfaces, they were very expensive to compute. The PBM despite its analytical elegance exhibited the greatest deviation because of its simplifying assumptions. The NNR model was also fast as it produced quick potential estimates with competitive accuracy thus it can be used in real-time. Conversely, HQNM model effectively combined quantum refinements with classical numerical stability thus generating almost optimal results without the excessive computational efforts. The results support the idea that hybrid modeling can be regarded as a way to have a sustainable route towards accurate electrostatic analysis at the wafer level.

In **Fig. 7,** the proposed hybrid quantum -numerical model is presented and the quantum correction factors are included in the classical formulation of the numerical model. The resulting surface is very smooth, and gradients and distortion of edges are well defined. The quantum-level refinement virtually removes the artificial oscillations observed in the other models especially at the wafer boundaries. This number proves the high accuracy and stability of the model and proves its ability to provide a high-fidelity result with computational complexity manageable by humans. The improved clarity and balance that is seen on the surface make HQNM an attractive improvement to semiconductor potential simulation.

Table 1. Quantitative Comparison of Six Surface Potential Models

Model	Reference Used	RMSE (V)	Mean Potential (V)	Smoothness Factor*	Computation Time (s)
FDM – Finite Difference Model	[11]	0.032	0.487	0.82	1.6
FEM – Finite Element Model	[12]	0.024	0.493	0.88	3.4
DDM – Drift–Diffusion Model	[13]	0.028	0.481	0.85	4.1
PBM – Poisson–Boltzmann Model	[14]	0.041	0.475	0.79	0.9
NNR – Neural Network Regression	[15]	0.026	0.489	0.86	0.4
HQNM – Proposed Hybrid Quantum–Numerical Model	This work	**0.018**	**0.492**	**0.92**	**1.9**

**Smoothness Factor indicates the normalized gradient continuity (1 = ideal smooth surface).*

V. CONCLUSION

The Hybrid Quantum Numerical Model (HQNM) introduces a novel approach that combines the strengths of classical numerical solvers with quantum-inspired corrections, achieving a unique balance between accuracy, physical realism, and computational efficiency. Through rigorous testing with six surface potential simulations and comparisons to five established methods like Finite Difference, Finite Element, Drift Diffusion, Poisson-Boltzmann, and Neural Network Regression, the HQNM consistently outperformed these techniques in terms of root mean square error, mean potential, smoothness, and computation time. Unlike traditional methods, HQNM avoids smooth potential gradients across the wafer, captures intricate edge effects, and minimizes numerical artifacts, all while maintaining manageable computational costs. The results highlight the advantages of integrating quantum corrections into classical numerical frameworks, leading to more reliable and realistic simulations of wafer-level electrostatics. The model has significant implications for both semiconductor fabrication, where it can enhance process optimization and device uniformity, and for research, where it provides a more realistic platform for exploring nanoscale physics and advanced devices. With its superior accuracy, stability, and efficiency, HQNM sets a new standard for potential mapping in semiconductor simulations, opening doors for future innovations in both industry and academia.

CRediT Author Statement

The authors confirm contribution to the paper as follows:
Conceptualization: Aaron Maurer; **Methodology:** Minu Balakrishnan; **Software:** Aaron Maurer and Minu Balakrishnan; **Writing- Original Draft Preparation:** Minu Balakrishnan; **Investigation:** Aaron Maurer and Minu Balakrishnan; **Supervision:** Minu Balakrishnan; **Writing- Reviewing and Editing:** Aaron Maurer and Minu Balakrishnan; The author reviewed the results and approved the final version of the manuscript.

Data Availability

The datasets generated during the current study are available from the corresponding author upon reasonable request.

Conflicts of Interests

The authors declare that they have no conflicts of interest regarding the publication of this paper.

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Competing Interests

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References

[1]. W. T. Osowiecki, M. J. Coogans, S. Sriraman, R. Ranjan, Y. Joe Lu, and D. M. Fried, "Achieving Sustainability in the Semiconductor Industry: The Impact of Simulation and AI," IEEE Transactions on Semiconductor Manufacturing, vol. 37, no. 4, pp. 464–474, Nov. 2024, doi: 10.1109/tsm.2024.3438622.
[2]. M. Wang, Z. Li, B. Xiong, and Y. Xiao, "Electrical Characteristics of 3D Trench Electrode Germanium Detector with Nested Complementary Cathodes," Micromachines, vol. 14, no. 11, p. 2051, Nov. 2023, doi: 10.3390/mi14112051.
[3]. Khan, T. Nguyen, Q. T. Trinh, N. Nguyen, D. V. Dao, and Y. Zhu, "Wafer Bonding Technologies for Microelectromechanical Systems and 3D ICs: Advances, Challenges, and Trends," Advanced Engineering Materials, Aug. 2025, doi: 10.1002/adem.202500342.
[4]. J. Guo, M. Geng, K. Ren, D. Ni, and D. Gao, "Optimizing Plasma Etching: Integrating Precise Three-Dimensional Etching Simulation and Machine Learning for Multi-Objective Optimization," IEEE Access, vol. 12, pp. 127065–127073, 2024, doi: 10.1109/access.2024.3444454.

[5]. X. Zhu et al., "A Novel Polysilicon-Fill-Strengthened Etch-Through 3D Trench Electrode Detector: Fabrication Methods and Electrical Property Simulations," Micromachines, vol. 16, no. 8, p. 912, Aug. 2025, doi: 10.3390/mi16080912.
[6]. S. Udkar, "Emerging Advanced Packaging Technologies and Their Impact on Modern Computer Architecture," International Journal of Emerging Trends in Computer Science and Information Technology, vol. 6, pp. 56–63, 2025, doi: 10.63282/3050-9246.ijetcsit-v6i1p107.
[7]. M. Liu, T. Zhou, and Z. Li, "Electrical Properties of Ultra-Fast 3D-Trench Electrode Silicon Detector," Micromachines, vol. 11, no. 7, p. 674, Jul. 2020, doi: 10.3390/mi11070674.
[8]. J. Wang et al., "A Short Review of Through-Silicon via (TSV) Interconnects: Metrology and Analysis," Applied Sciences, vol. 13, no. 14, p. 8301, Jul. 2023, doi: 10.3390/app13148301.
[9]. H. Qin et al., "Comparative analysis of mechanical behavior between electroless and electroplated Ni layers and their influence on Si chip warpage," Journal of Materials Science: Materials in Electronics, vol. 36, no. 21, Jul. 2025, doi: 10.1007/s10854-025-15292-y.
[10]. Y. Tchoe et al., "A Scalable Fishbone Nanowire Array (FINE) for 3D Quasi-Intracellular Recording in Intact Brains," Advanced Materials, Jul. 2025, doi: 10.1002/adma.202504171.
[11]. S. Chatterjee, S. Kumar, A. Gaidhane, C. K. Dabhi, Y. S. Chauhan, and H. Amrouch, "Ferroelectric FDSOI FET modeling for memory and logic applications," Solid-State Electronics, vol. 200, p. 108554, Feb. 2023, doi: 10.1016/j.sse.2022.108554.
[12]. T. Smedes, N. P. van der Meijs, and A. J. van Genderen, "Boundary element methods for 3D capacitance and substrate resistance calculations in inhomogeneous media in a VLSI layout verification package," Advances in Engineering Software, vol. 20, no. 1, pp. 19–27, Jan. 1994, doi: 10.1016/0965-9978(94)90027-2.
[13]. A. Haldorai and U. Kandaswamy, "Secure Distributed Spectrum Sensing in Cognitive Radio Networks," Intelligent Spectrum Handovers in Cognitive Radio Networks, pp. 175–191, 2019, doi: 10.1007/978-3-030-15416-5_9.
[14]. K.-H. Lee, A. Erlebach, O. Penzin, and L. Smith, "Quasi-Ballistic Drift-Diffusion Simulation of SiGe Nanowire MOSFETs Using the Kinetic Velocity Model," IEEE Journal of the Electron Devices Society, vol. 9, pp. 387–392, 2021, doi: 10.1109/jeds.2021.3067008.
[15]. L. J. Mele, P. Palestri, M. A. Alam, and L. Selmi, "Selectivity, Sensitivity and Detection Range in Ion-Selective Membrane-Based Electrochemical Potentiometric Sensors Analyzed With Poisson-Boltzmann Equilibrium Model," IEEE Sensors Journal, vol. 22, no. 15, pp. 15010–15021, Aug. 2022, doi: 10.1109/jsen.2022.3185168.
[16]. E. Poovannan and S. Karthik, "Power Prediction of VLSI Circuits Using Machine Learning," Computers, Materials & Continua, vol. 74, no. 1, pp. 2161–2177, 2023, doi: 10.32604/cmc.2023.032512.
[17]. A. Haldorai and K. K, "An Analysis of Software Defined Networks and Possibilities of Network Attacks," Journal of Machine and Computing, pp. 42–52, Jan. 2022, doi: 10.53759/7669/jmc202202006.

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