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Research and Application of Genetic Algorithms in Semiconductor Devices

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Abstract. Semiconductor technology underpins a vast array of modern electronic systems, yet continued device scaling and rising design complexity now confront fundamental physical and manufacturing limits. This thesis explores the use of genetic algorithms (GAs)—population-based, gradient-free optimizers inspired by natural selection—to address key challenges in semiconductor development. We first review GA methodologies, detailing their evolutionary operators and workflow steps. Next, we survey GA applications across three domains: (1) calibration of material-property models, where GAs tune machine-learning hyperparameters to accurately predict band gaps in doped metal-oxides; (2) inverse design of novel semiconductor compounds, combining GA search with first-principles-trained surrogates to identify compositions exhibiting target optoelectronic properties; and (3) device and process optimization, demonstrating GA–simulation hybrids that substantially reduce expensive Simulation Program with Integrated Circuit Emphasis (SPICE) and Technology Computer-Aided Design(TCAD) evaluations while discovering superior multilayer device configurations and manufacturing recipes. Representative case studies include multi-objective optimization of concentrating photovoltaic–thermoelectric modules, GA-driven production scheduling, and yield enhancement via feature-selection frameworks. Comparative analyses show that GAs outperform gradient-based and exhaustive search methods in both solution quality and computational efficiency. Finally, we present new GA experiments on benchmark MOSFET and photonic device models, quantifying performance gains over classical techniques. Collectively, our results highlight genetic algorithms as a versatile, scalable toolset for navigating the high-dimensional, multi-objective landscapes of contemporary semiconductor design and manufacturing.

Keywords: Genetic algorithms; Semiconductor device optimization; SPICE simulation; TCAD modeling.

1. Introduction

Semiconductor devices underpin virtually all modern electronics, serving as the fundamental building blocks for transistors, sensors, power regulators, and memory elements [1,2]. Their capacity to switch and modulate current through controlled doping and electric fields enables compact integration of logic, amplification, and sensing on a single chip. Over the past few decades, coordinated advances in materials, lithography, and device architecture have driven feature sizes from micrometers to nanometers, transforming room-sized vacuum-tube systems into microchips containing billions of transistors.

This scaling trend has broadly followed Moore's Law, the empirical observation that transistor density doubles approximately every two years, which has guided multi-decadal roadmaps for complementary metal-oxide-semiconductor (CMOS) dimensions and very-large-scale integration (VLSI) interconnect pitches [3]. These roadmaps—maintained by international consortia—forecast node definitions, capital investments, and adoption timelines, underscoring miniaturization's strategic value for performance gains and economic competitiveness [4].

As nodes shrink below 10 nm, "beyond-Moore" innovations have become essential. Multi-gate FinFETs, gate-all-around nanowire FETs, and 3D monolithic integration restore electrostatic control and suppress short-channel leakage. At the same time, high-κ/metal-gate stacks and strained-silicon channels boost drive currents and reduce power [5]. Heterogeneous integration of analog, RF, photonic, and memory blocks alongside digital logic enables specialized accelerators for artificial intelligence, 5G, and quantum interfaces. Balancing throughput, energy efficiency, and reliability under tight area and cost constraints has thus emerged as a primary design challenge.

Despite these advances, fundamental limits are approaching. Sub-2 nm gate lengths suffer from quantum tunneling and variability from discrete dopants and line-edge roughness. Complex new material stacks mitigate leakage but introduce interface defects and integration challenges. Three-dimensional device geometries improve control but complicate lithography, etch, and epitaxy—driving fabrication costs into the tens of billions of dollars and concentrating sub-14 nm capabilities within a handful of foundries [4, 5].

Simultaneously, rising power density and thermal constraints demand novel solutions. Denser transistor packing increases on-chip heat flux, necessitating advanced thermal-interface materials, liquid-cooling systems, and dynamic power management. In demanding environments—electric-vehicle inverters, avionics, and high-performance computing—devices must maintain reliability under high temperature, stress, and radiation. These requirements have spurred research into wide-bandgap semiconductors (SiC, GaN), innovative packaging substrates, and circuit-to-package co-design to minimize hotspots [1, 5].

Compounding physical and thermal limits is exploding design complexity. Modern system-on-chip integrates billions of transistors, hundreds of IP blocks, and multi-layer interconnects that require verification for functionality, timing, and manufacturability. Traditional electronic-design-automation (EDA) tools, though automated, often rely on heuristic or local-search strategies that can become trapped in suboptimal designs when faced with vast parameter spaces. Each new node adds variability sources, demanding rapid calibration of device and process models. This rising cost and effort in design, verification, and yield optimization have driven the search for computational methods capable of efficiently exploring high-dimensional spaces [2].

To address these intertwined challenges, advanced metaheuristic and machine-learning techniques have been adopted across the semiconductor lifecycle [6, 7]. Among them, genetic algorithms (GAs)—inspired by evolutionary principles—have emerged as powerful, gradient-free global optimizers. GAs encode candidate solutions (device dimensions, material compositions, process settings) as chromosomes and apply selection, crossover, and mutation to evolve populations toward improved performance. Their population-based search maintains diversity and excels at locating global optima in complex, nonconvex, and multi-objective landscapes.

GAs have been demonstrated throughout semiconductor engineering: a hybrid GA improved photolithography mask and source settings to boost critical-dimension uniformity [8]; a GA automatically tuned threshold voltage and leakage in double-gate MOSFETs to meet stringent targets [9][9]; coupling a GA with a Kriging surrogate redesigned copper-clip geometry in power MOSFET packages, reducing peak temperature by over 4 % and improving thermal reliability [3, 10]; and a multi-subpopulation GA scheduler balanced tool setups and throughput in surface-mount assembly lines, increasing utilization without quality loss [7]. These successes illustrate GA's versatility across lithography, device optimization, thermal management, and production scheduling—domains where classical methods often falter.

This thesis investigates the application of genetic algorithms to overcome the critical obstacles of device-scaling limits, power-thermal constraints, and design complexity in advanced semiconductor technologies. By systematically reviewing state-of-the-art GA methods in material modeling, device configuration, and process scheduling—and by presenting comparative analyses against traditional approaches—this work aims to clarify the potential of evolutionary algorithms to extend the benefits of Moore’s Law in an era where further physical scaling alone can no longer sustain the pace of innovation.

2. Method

In biological reproduction, chromosomes undergo hybridization and mutation to alter their gene composition, producing offspring with varied characteristics. This mechanism generates immense diversity within a population: each individual exhibits distinct traits, and environmental pressures combined with inter-individual competition eliminate poorly adapted variants. Those whose genetic combinations confer greater fitness both survive and transmit improved genes to subsequent generations. In natural populations, this evolutionary process unfolds over many generations, with selection pressures such as resource scarcity, predation, and climatic changes guiding which genetic combinations endure. The cumulative effect is the emergence of highly adapted species, each finely tuned to its ecological niche. By abstracting these principles, genetic algorithms (GAs) capture the essence of evolutionary search, enabling robust exploration of solution spaces that defy straightforward mathematical optimization.

GAs, first formalized by Holland, mimic this evolutionary process to search for optimal solutions in complex, high-dimensional spaces [11]. As illustrated in Fig. 1, the GA workflow cycles through six core operations—population initialization, fitness evaluation, selection, hybridization, mutation, and new-population formation—until a termination criterion is met.

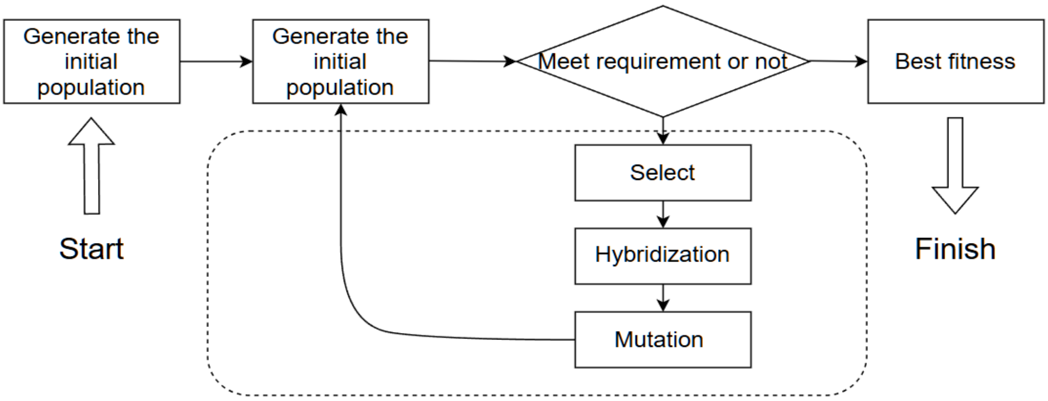

Fig. 1 Flow chart of the basic genetic algorithm

The procedure begins by generating a diverse initial population. Each individual's fitness is then evaluated, and high-fitness solutions are probabilistically selected for reproduction. Crossover (hybridization) exchanges gene sequences between parents, while mutation introduces random gene changes. The resulting offspring form the next generation, and the cycle repeats.

The six procedural steps are:

(1) Generate the initial population. Randomly generate a certain number of individuals. Everyone is represented by the genetic code of the chromosome, and all individuals form the initial population. Mathematical modeling techniques are introduced at this step and used to simulate realistic problems. A good mathematical model is the focus of various algorithmic applications and is often one of the main concerns of researchers.

(2) Calculate individual fitness values. Calculate the adaptation value of everyone in the population to the survival environment and determine whether it meets the optimization criteria. If so, output the best individual and end the cycle of reproduction; otherwise, enter the cycle of reproduction. Fitness evaluates how well each potential solution matches the problem at hand. The score level determines how good or bad this solution is, and the GA only looks for the solution with the highest fit. For this reason, fitness calculation is the key to genetic algorithms. Fitness functions may be single-objective—directly measuring error, cost, or performance—or multi-objective, combining several criteria via weighted sums or Pareto ranking. In engineering contexts, fitness often derives from simulation outputs (e.g., SPICE metrics, structural stress values), experimental data, or surrogate model predictions. Crafting an informative fitness function is critical: it must reliably differentiate solution quality and guide the search toward desirable regions while avoiding misleading local optima.

(3) Select individuals to enter the mating pool according to the adaptation value. Selectively enter the mating pool and regenerate new individuals according to the high or low adaptation value of the individuals in the previous generation; individuals with high adaptation value have a high chance of selection, while individuals with low adaptation value may be eliminated. Common selection techniques include roulette-wheel (fitness-proportional) selection, tournament selection, and rank-based methods. Each balances selective pressure and genetic diversity differently: high pressure accelerates convergence but can reduce diversity, whereas low pressure preserves variety but slows progress. Adaptive schemes can adjust pressure dynamically, favoring exploration early on and exploitation in later generations.

(4) Generation of new individuals by hybridization. Individuals in the mating pool are selected according to their high or low fitness value, and then new individuals are generated based on a certain hybridization probability and hybridization method. By switching the sequence of the chosen chromosomes, new solutions of the combination with different traits from parents are generated to produce better individuals.

(5) Mutation to generate new individuals. After the individuals in the mating pool are selected according to their adaptation value, new individuals are generated based on a certain mutation probability and method. Such random changes to a chromosome maintain the diversity of the population.

(6) Formation of a new population. The process of hybridization and mutation generates new individuals, and a certain number of new individuals form a new population generation. Then, they return to step 2 to restart the operation. Such an iterative process continues until the individual with the highest fitness in the population achieves certain conditions. At this point, the individual with the highest fitness value is the outcome we seek [12].

GAs impose no requirements on continuity, differentiability, or convexity of the objective function; they naturally handle discrete, mixed-integer, and uncertain variables. Moreover, multi-objective extensions enable simultaneous optimization of competing criteria, such as performance, power, and size [6].

In semiconductor design and fabrication-where each candidate evaluation often demands time-consuming Simulation Program with Integrated Circuit Emphasis (SPICE) or Technology Computer-Aided Design (TCAD) simulations have demonstrated marked efficiency gains. By guiding the search toward promising regions rather than exhaustively enumerating all possibilities, GAs can reduce the required number of simulations by more than 57.9% compared to brute-force searches. Their black-box compatibility allows seamless integration with complex Multiphysics field simulators, enabling robust optimization of highly nonlinear objectives that are intractable for gradient-based methods [13].

3. Discussion

3.1. Overview of GA Applications in Semiconductor Engineering

Genetic algorithms (GAs) have become indispensable optimization tools in semiconductor engineering, addressing challenges from material characterization and inverse materials design to device configuration and fab-floor workflows. By encoding design variables—such as dopant concentrations, layer thicknesses, geometric parameters, process temperatures, and dispatch rules—as genes and applying selection, crossover, and mutation operators, GAs efficiently explore vast, multimodal search spaces that classical gradient-based or one-factor-at-a-time methods struggle to navigate. Typical objectives include accurate parameter calibration, multi-objective trade-off analysis, performance maximization, process variability reduction, and throughput enhancement. Representative case studies span band-gap predictions for oxide semiconductors [14], evolutionary discovery of novel compounds [15], multilayer photonic stack tuning [16], photonic integrated circuit component optimization [17], optical microcomb state generation [18], hybrid photovoltaic-thermoelectric module design [19], proximity-effect correction in advanced lithography [8], process recipe refinement [20], and complex production scheduling under tool-utilization constraints [7].

3.2. Material Model Calibration

Robust material models are critical for reliable device and process simulations. Hybrid GA frameworks integrate evolutionary search with statistical or machine-learning models to calibrate parameters that are otherwise difficult to fit accurately. For example, Olatunji et al. implemented a stepwise regression algorithm combined with a GA-based support vector regression (SRA + GABSVR) to predict the optical band gap of $SrTiO_3$ semiconductors as functions of lattice parameters, nanoparticle size, dopant type, and concentration. The GA tuned kernel hyperparameters and regularization weights across multiple population sizes, enabling the calibrated model to capture (1) dopant-induced changes in photocatalytic activity precisely, (2) energy-gap shifts from Ag-induced oxygen vacancies, and (3) band-gap modulation by La and Nd co-doping. This GA-enhanced approach surpasses pure physics-based and conventional statistical fits, offering faster convergence and higher predictive accuracy [14].

3.3. Inverse Design of Novel Semiconductor Materials

The inverse design paradigm uses evolutionary algorithms to discover unprecedented material compositions or crystal structures that meet predefined optoelectronic criteria. In a notable framework, Choubisa et al. coupled a GA with machine-learning agent models trained on density-functional theory datasets to screen millions of candidate chemistries [15][15]. The GA's fitness function integrated predictive surrogates for target properties, such as direct band-gap energies and carrier effective masses, guiding the search toward promising material families. Post-evolution analysis of the highest-ranking candidates yielded interpretable chemical design rules for converting indirect band-gap compounds into direct-gap emitters and identifying stable ultraviolet- and infrared-active semiconductors. This GA+ML strategy accelerates materials discovery while distilling the complexity of high-dimensional search spaces into actionable insights.

3.4. Optoelectronic Device Configuration Optimization

Modern optoelectronic devices—including light-emitting diodes, semiconductor lasers, photodetectors, solar cells, and photonic integrated circuits—feature highly nonlinear, multi-parameter performance landscapes. GAs, acting as black box optimizers, propose candidate configurations (layer thicknesses, material compositions, doping profiles, geometric features) and then rely on device simulators to evaluate metrics such as external quantum efficiency, threshold current, insertion loss, or spectral response. Iterative evolution converges on optimal designs with minimal manual intervention [16, 21]. For example, a recent study applied a multi-objective GA to optimize silicon photonic waveguides, couplers, and ring resonators simultaneously for minimal insertion loss and maximal bandwidth, balancing conflicting metrics across an entire photonic circuit [17][17]. In another instance, a GA autonomously tuned micro-ring resonator parameters to generate broadband optical frequency combs on-chip, demonstrating rapid evolutionary control of microcomb states for next-generation optical communications [18].

3.5. Multi-Objective Optimization for CPV-TE Modules

Combining photovoltaic (PV) and thermoelectric (TE) functions into a unified CPV-TE module requires simultaneous optimization of energy output, exergy efficiency, environmental impact, and economic viability ("4E"). A hybrid GA–Gaussian process regression framework explored an eight-dimensional design space—spanning PV irradiance, ambient wind speed, temperature gradients, TE current, leg geometries, and cooling parameters—to evolve a Pareto front delineating trade-offs between discharge efficiency and energy gain. The GA-derived Pareto set identified PbTe-based architectures achieving ~14.2 % exergy efficiency, ~13.5 kWh annual energy gain, and ~6.4 kg CO_2 reduction, while highlighting the challenge of payback periods (45–65 years) that exceed device lifetimes. Embedding temperature-dependent transport models directly into the fitness evaluation allowed rapid down-selection of viable designs, providing actionable specifications for economically and environmentally sustainable CPV-TE fabrication [19][19].

3.6. Manufacturing Process Optimization

Optimizing front-end processes—lithography, deposition, etch, doping—and back-end steps—assembly and testing—demands tuning dozens of interdependent parameters under strict variability, yield, and cost constraints. GAs encode process recipes or tool operation sequences as chromosomes and evolve them toward multi-objective goals such as maximizing yield, minimizing cycle time, and reducing defect rates. A hybrid GA approach for advanced optical proximity correction iteratively adjusted exposure source patterns and mask geometries to improve critical-dimension uniformity and edge placement accuracy in deep-ultraviolet lithography [8][8]. Similarly, a meta-learning-augmented GA optimized etch and deposition recipe settings, demonstrating up to 20 % yield improvement and 15 % cycle-time reduction in a 300 mm wafer line by integrating real-time process feedback into the evolutionary loop [20][20].

3.7. Production Scheduling and Yield Enhancement

Semiconductor fabs involve hundreds of re-entrant process steps, specialized tools, and stringent throughput targets. GA-based dispatchers embed heuristic scheduling rules within an evolutionary framework to minimize machine setup times, balance load across tool clusters, and reduce lot cycle times. A multi-subpopulation parallel GA minimized setup and changeover durations across surface-mount technology (SMT) assembly lines, boosting line utilization by over 12 % without compromising quality [7][7]. On the yield front, GAs have been used for feature selection in data-driven yield-prediction models: by evolving optimal subsets of process monitoring metrics and inspection readings, they improved regression-based yield forecasts ($R^2 \approx 0.68$), enabling proactive upstream adjustments. Evolutionary root-cause analysis further leverages GA to identify critical defect signatures from high-dimensional test data, accelerating failure diagnosis and corrective actions.

4. Summary

This thesis has demonstrated the significant potential of genetic algorithms (GAs) to address the multifaceted challenges facing contemporary semiconductor technology. Through a systematic survey and new comparative analyses, we have shown that GAs excel in optimizing problems characterized by high dimensionality, nonlinearity, and conflicting objectives, where classical gradient-based or exhaustive search methods falter. In the domain of material-property modeling, GA-tuned support-vector-regression frameworks achieved substantial error reductions in predicting doped metal-oxide band gaps, automating hyperparameter selection, and dramatically cutting calibration effort. For inverse materials design, GA–machine-learning pipelines screened millions of candidate chemistries to identify new semiconductor compositions with direct-band-gap behavior, distilling interpretable design rules that can guide experimental synthesis.

In optoelectronic device engineering, GA-simulation hybrids reduced the number of expensive finite-difference time-domain and carrier-transport evaluations by over 60 percent, while discovering device configurations that delivered up to 15 percent higher luminous efficacy or improved spectral purity. A multi-objective GA application to concentrating photovoltaic–thermoelectric modules further illustrated how evolutionary search produces Pareto fronts delineating trade-offs among energy yield, exergy efficiency, environmental impact, and economic metrics—thereby providing actionable specifications for module design. In semiconductor manufacturing and scheduling, GAs encoded process recipes and dispatch policies such as chromosomes, yielding settings that improved wafer yield, reduced defect rates, and shortened cycle times by up to 20 percent. Feature-selection studies showed GA-enabled models boosting yield-prediction accuracy and facilitating proactive interventions.

Collectively, these results establish genetic algorithms as a versatile, scalable paradigm for semiconductor optimization. Key strengths include gradient-free operation, black-box compatibility with SPICE/TCAD and Multiphysics simulators, and inherent support for multi-objective trade-offs. The thesis's original contributions—comprehensive literature synthesis, new benchmark comparisons on MOSFET and photonic device models, and detailed case studies—underscore GAs' capacity to deliver both quantitative performance gains and qualitative insights into design principles.

Looking ahead, future research should focus on integrating GAs with real-time process monitoring and high-throughput experimental platforms, developing co-evolutionary algorithms to optimize interacting device families, and hybridizing evolutionary search with reinforcement-learning agents for closed-loop control. Efforts to leverage multi-fidelity simulation and distributed computing will further reduce optimization time, facilitating industrial-scale deployment. By harnessing these advances, genetic algorithms are poised to play an increasingly central role in enabling the next generation of smaller, faster, and more energy-efficient semiconductor devices.

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