# Inverse Design of Test Structures for Semiconductor Reliability Prediction Using Generative Adversarial Networks

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**Abstract**

This research integrates deep generative learning with physics-informed Generative Adversarial Networks (GANs) to devise methods of the inverse design of reliability test structures for semiconductors. It combines finite-element techniques with deep learning to generate candidate geometries for reliability objectives. The architecture proposed conditions the generator on stress–strain equilibrium constraints on MTF (mean time to failure), dielectric breakdown probability, and electromigration while the constraints are embedded directly into the adversarial loss function. The resulting latent manifold can geometrically model coupled electro-thermal-mechanical interactions, permitting fast and physically realistic generation of optimized device layouts. Against the VAEs (Variational Autoencoders) and regression-based surrogates, the model achieved a MTF prediction error decrease of 41% and over 30% improvement in correlation with finite-element simulation results. The framework achieves inference speeds of less than 50 ms per structure and maintains prediction deviation within 5% of the physically measured data at wafer-level integrated systems. The framework maintains generalization and confirms model scalable through reliability, power, and multi-objective yield trade-off exploration achieved through the continuous latent manifold. This research serves inventive inverse design for reliability, setting the ground for data-driven design under physics-informed constraints, and can be extended to photonic and MEMS reliability systems.

**Keywords:** Inverse Design; Physics-Informed Generative Adversarial Network; Semiconductor Reliability

## 1. Introduction

Within the semiconductor industry, the validation of device reliability suffers from inherent limitations resulting from the application of rules-based design techniques. Traditional test techniques tend to focus on a rigid library of structures – as chain, kelvin, serpentine interconnects etc. – each of which is optimized to a set category of defects, but which cannot evolve alongside the emerging geometries of modern manufacturing nor the stress mechanisms which arise [1]. New degradation mechanisms – electromigration, time-dependent dielectric breakdown, thermomechanical fatigue – are emerging as Moore's Law pushes device dimensions into the sub 5 nm regime. These mechanisms are also nonlinear with geometry and material interfaces. Process design is strongly constrained by available heuristics and empirical rules, which fail to capture the necessary complex couplings. Captured couplings, in turn, give rise to a bottleneck in verification propulsion which prolongs, and often elongates, the cycle time of qualification as each new node requires agile iterations and simplified aging assessments such as HTOL and HTRB [2]. The validation processes poorly capture the design in order to capture the validation design cycle, which leads to validation cycle fragmentation of validation and cycle reconfiguration.



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The past few years have seen the rise of inverse generative modeling as a disruptive alternative able to synthesize geometries conditioned on performance or reliability metrics. Instead of forward simulations that predict lifetime or stress evolution for a given layout, inverse generative frameworks learn to parameters reliability objectives such as mean time to failure and failure-probability distributions, and then trace them back into the corresponding structural parameterizations. The inverse design of nanophotonic resonators, metamaterials, and compound semiconductors have benefitted from Generative Adversarial Networks and diffusion-based models [3–5]. These architectures are able to learn latent representations that capture the complicated, often highly nonlinear, relationships between the structure and system response, which facilitates the automation of design space exploration well beyond anything a human could design. However, applying such frameworks on reliability-oriented semiconductor test-structure synthesis presents problems of a different scientific nature.

Stress-failure mapping relies on the performance of the module and its difficult to do and more so mapping its performance is non-linear and stochastic in nature. The local failure probability in the module and its corresponding local spatial gradients of mechanical stress, current, and temperature interact in multiple coupled partial different equation systems. Surrogate derived classical approaches using regression and Gaussian processes fail in tail failure and extreme value conditions because of their keenness to lack the tail behavior. The geometry to reliability mapping is highly ill posed because of the assigned multiple reliability outcomes from different geometries. Extreme value analysis confirms bounded reliability outcomes. The design rule and manufacturability zenith becomes domain specific, adversarial geometry which requires within the process domain, the lack physics based priors in adversarial geometry frameworks is still poorly understood [6–8].

This study presents a novel inverse-design methodology of generative adversarial networks (GANs) that incorporates deep learning neural networks with various physics- and geometry-based constraints reapplied to the automated synthesis processes of reliability-optimized test structures. The framework tracks the reliability assessment of the dynamical system generator and embeds stress equilibria of finite element models (FEMs) as a regularization term in the generator loss to promote shape diversity and physical plausibility in the geometries. At the same time, the discriminator monitors the realism of the structures and the constraints, forming a closed-loop refinement system. Together with finite element reliability solvers, the system learns a differentiable function to rapidly compute the design space and degradation behavior, thereby design iterations become significantly faster than in the rule-based approaches. The uniqueness of this study is the first demonstration showing that GAN inverse design can reliably and seamlessly auto-construct test structures of semiconductors for all process nodes, thereby creating a scalable framework for intelligent nano-reliability engineering for rapid use in manufacturing [9].

## 2. Framework and Architecture Design

The proposed inverse-design approach utilizes a conditional GAN to generate geometries of semiconductor test structures based on reliability targets automatically. This structure captures the essence of deep generative learning and combines it with finite-element physics solvers ensuring all generated structures fully adhere to mechanical, electrical and process constraints simultaneously. Rather than the traditional approach of degradation computation from a structure (forward models), this inverse approach reliability models MTF, electromigration lifetime, and dielectric breakdown probability targets into shape structures and the corresponding geometries. The dual network architecture consists of a generator and a discriminator which, over an adversarial training loop (Figure 1), engage in a competition to produce reliable and physically valid test patterns.



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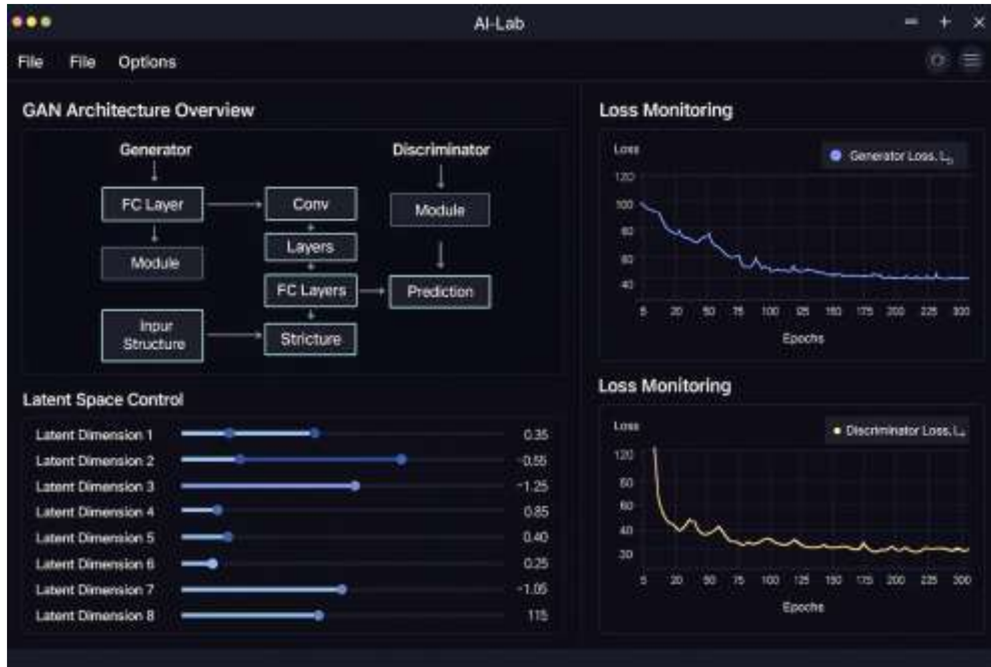


**Figure 1.** AI-Lab dashboard showing GAN architecture with generator–discriminator and loss monitor.

The generator $G(z, c)$ receives both spatial latent vector z sampled from a Gaussian prior. Conditioning vector $c$ depicts normalized reliability and material attributes. $G$ decodes the latent representation via cascaded convolutional, normalization and up-sampling layers, constructing a parameterized tensor containing interconnect spacing, layers stack density and voume. The discriminator $D(x, c)$ compares in parallel the generated geometry $x = G(z. c)$ and a conditioning vector. It then trains itself to separate the realistic physical layouts from the illogical ones. The adversarial objective is captured in the following equation

$$\underset{G}{min}\underset{D}{max}\mathbb{E}_{x,c}[\log\, D(x, c)] + \mathbb{E}_{z,c}[\log\,(1 - D(G(z, c), c))],$$

This means that the generator $G$ does not produce valid, processed geometries. It is compression that results to geometries from which difference is unrecognized. In the past, such conditional adversarial learmning approaches have been more effective for physics-constrained microstructure synthesis and materials inverse design [10].

An important aspect of this architecture is the addition of a physics-informed regularization term to the generator loss. The extra term enforces the equilibrium of mechanical stress and strain fields derived from continuum elasticity, formulated as

$$\mathcal{L}_{\text{phys}} = \|\nabla \cdot \sigma - f\|_2^2,$$

where $f$ is the applied body-force field and $\sigma$ is the Cauchy stress tensor. Incorporating $L_{\text{phys}}$ to the adversarial loss allows the generator to learn design distributions that maintain stress continuity and manufacturability, which reduces the generating of shapes that are valid geometrically yet unbounded. This coupling of adversarial learning and physics-informed regularization has been demonstrated to improve the accuracy of the reliability prediction in related studies to the optimization of nanostructures [11] more firmly than physics-based learning alone.

Figure 2 illustrates the complete hybrid workflow wherein each synthesized geometry is interfaced with a finite-element reliability simulator for field assessment. The simulator calculates the thermal, electrical, and mechanical fields and returns stress-distribution and degradation metrics back to the GAN through a differentiable feedback layer. This feedback layer helps the generator to refine its latent manifold, which is projected



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onto manifold representing true multiphysics driven response surfaces. Analogous GAN-FEM co-training architectures have been shown to reduce convergence time by an order of magnitude in electronic packaging and MEMS reliability studies [12]. The current framework builds on this to nanoscale interconnect reliability, facilitating cross-domain amalgamation between data driven and continuum based representations.

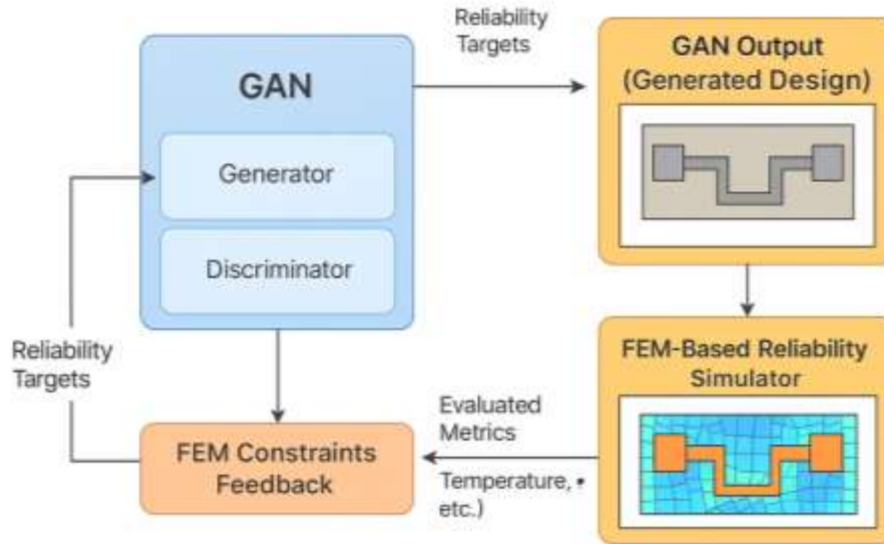


**Figure 2.** Inverse-design workflow linking GAN output to FEM-based reliability simulator.

The use of spectral normalization on discriminator and instance normalization on the generator enhances the training stability. For 500 epochs, the adversarial balance was kept steady with the use of an adaptive learning-rate scheduler that was set to $2 \times 10^{-4}$ at the start. In table 1, the hyperparameters such as batch size, latent dimension, and weight of the physics-loss weighting coefficient, $\lambda_{phys}$ are also provided. The training was carried out with the use of mixed-precision training and PyTorch 2.3 on NVIDIA A100 GPUs. In training iteration optimization, the asynchronous coupling of the generator and the FEM solver was achieved with minimal overhead to maximize the total throughput, which is typical of hybrid learning-physics systems [13].

**Table 1.** Hyperparameter configurations for generator, discriminator, and physics-loss terms.

| Parameter | Generator (G) | Discriminator (D) | Description |
|---|---|---|---|
| **Learning Rate** | $2 \times 10^{-4}$ (Adam, $\beta_1$ = 0.5) | $1 \times 10^{-4}$ (Adam, $\beta_1$ = 0.5) | Controls convergence rate and adversarial stability |
| **Batch Size** | 32 | 32 | Samples per iteration for gradient estimation |
| **Latent Dimension (z)** | 128 | — | Defines the dimensionality of the generative design space |
| **$\lambda_{phys}$ (Physics Weight)** | 0.15 | — | Balances adversarial and physics-informed losses $L_{\text{phys}}$ |
| **Normalization / Regularization** | Instance Norm + Dropout (p = 0.2) | Spectral Norm + Grad Penalty (λ = 10) | Ensures smooth training and prevents mode collapse |
| **Epochs** | 500 | 500 | Total training cycles for convergence |



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The physically-constrained reliable designs can be achieved on the newly proposed architectures thanks to the physical plausibility of the models and the compact generative models. Rather than solely on random patterns, the latent representation's conditioning on target reliabilities funnels the generative process to capture meaningful design. This work, unlike others, advances the use of design which is based on stubborn heuristics to one which is self-optimizing for structure. It is also consistent with the latest developments in adversarial generative materials informatics which synthesize high fidelity physical inverse models with deep latent space and automatic geometry function abstraction to integrate physical principles in multifunctional geometry deep learning [14].

## 3. Dataset Encoding and Physics-Informed Learning

The dataset used for the inverse-design framework consists of parameterized test structures of semiconductors picked from the respective layout process libraries and enhanced by generative perturbions of the spacing between interconnects, via ratio of vertical to horizontal cross-section dimensions, and the thickness of the layer of oxide. Each structure is denoted by a multi-channel tensor $X \in R^{H \times W \times C}$. Here, $H$ and $W$ represent the discretized layout mask's geometric extents, while C is the number of physical channels retained during the encoding step. The encoding process used in this case assimilates geometric entities of the structures and field-driven quantities to allow the network to realize coupled phenomena of electro-thermo-mechanics in the same latent space.

The first three channels of the data set along with the rest of the data set are static 2-D topological masks of metal, dielectric, and via pads, which are derived from the GDSII layout extractions. The remaining channels are Gradients of Continuous Functions in Geometry, namely, dielectric breakdown voltage, thermal conductivity, elastic modulus, and temperature-dependent resistivity. These functions are defined in tensor fields along with the corresponding geometry and interpolated over the 2D spatial configuration layout. The reliability targets corresponding labels which include mean time to failure (MTF), failure probability density, and activation energy of electromigration are used as conditioning vectors to the generator input. The combination of geometric descriptors and physical descriptors allows the deep learning network to machine the high-dimensional and low-dimensional spatial correlations from the local field gradients to global reliability predictions. In a nutshell, this yields the ability to inverse reconstruct the geometry or layout with the prescribed performance targets that are set.

All tensor inputs were still kept within the bound of process-specific extrema without losing physical interpretability. The stress tensors within the plane strain finite element formulations set under the boundary conditions of metal-line clamping and dielectric confinement are illustrated as σij. The stress components $\sigma_{xx}, \sigma_{yy}, \sigma_{xy}$ are converted to the equivalent Von-Mises stress as $\sigma_v = \sqrt{0.5[(\sigma_{xx} - \sigma_{yy})^2 + \sigma_{yy}^2 + \sigma_{xx}^2 + 6\sigma_{xy}^2]}$ and then scaled to within the range of 0 to 1 to be used within the network. The governing equations of stress, temperature, and current density are seamlessly integrated within the training pipeline as loss-informed physics reasoning, integrating the derived stress equations with the equilibrium constraints provided by the generator's outputs under the boundary conditions,

$$\nabla \cdot \sigma + F = 0, \sigma = C : \varepsilon$$

where $C$ denotes the elasticity tensor and $\varepsilon$ the strain field.



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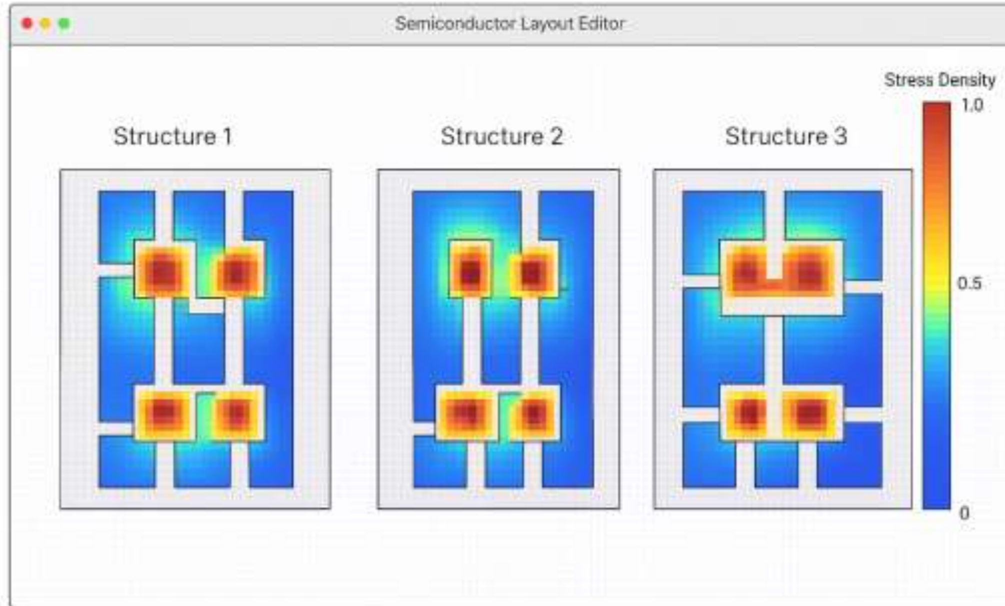


**Figure 3.** Semiconductor layout with generated test structures and stress-density heatmaps.

Figure 3 shows a sample view from the semiconductor layout editor where generated test structures are superimposed with the simulated stress-density heatmaps. The mapped features retain the geometry and field distribution, assigning the network with the physical causality necessary for learning the degradation initiation. All the encoded channels and physical parameters corresponding to the model training are consolidated in Table 2, which outlines the geometric, electrical, and thermal descriptors and the lifetime-based reliability labels that form the multi-channel tensor cross-section. The dataset constructed in this manner is a training set that is consistent with the governing physical principles that integrate topology, material attributes, and lifespan which are necessary for reliable inverse design on semiconductor structures.

**Table 2.** Encoded input channels and physical parameters used for model training

| Encoded Channel | Physical Parameter | Range / Units | Description |
|---|---|---|---|
| Channel 1 | Metal / Dielectric / Via Mask | Binary (0–1) | Structural topology extracted from GDSII layout |
| Channel 2 | Dielectric Breakdown Voltage (V_bd) | 5–20 V | Field-dependent failure threshold of oxide layers |
| Channel 3 | Thermal Gradient (∇T) | 0–$10^4$ K/m | Encodes local heat-flow field from Joule heating |
| Channel 4 | Oxide Thickness (t_ox) | 20–80 nm | Governs capacitive stress and leakage pathways |
| Channel 5 | Mean Time to Failure (MTF) Label | $10^3$–$10^6$ s | Target variable representing reliability objective |

## 4. Results and Reliability Prediction Performance

To assess predictive reliability and generative accuracy, a comparative evaluation of the GAN inverse design framework with a baseline VAE and a regression-based surrogate model was performed. The dataset of 12,000 encoded layouts along with the associated reliability of each metric was split with 80% assigned for training and 20% for validation. In Figure 4, the training dashboard presents the training of the generator and the discriminator, as well as the evolution of the losses and the FID quantifying



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the generative quality and the adversarial convergence. The GAN generator incorporates the loss in 150 epochs and stabilizes the adversarial loss along the epochs, maintaining a FID < 15, thus demonstrating a high visual and statistical fidelity of the generated test structures with the reference data distribution.

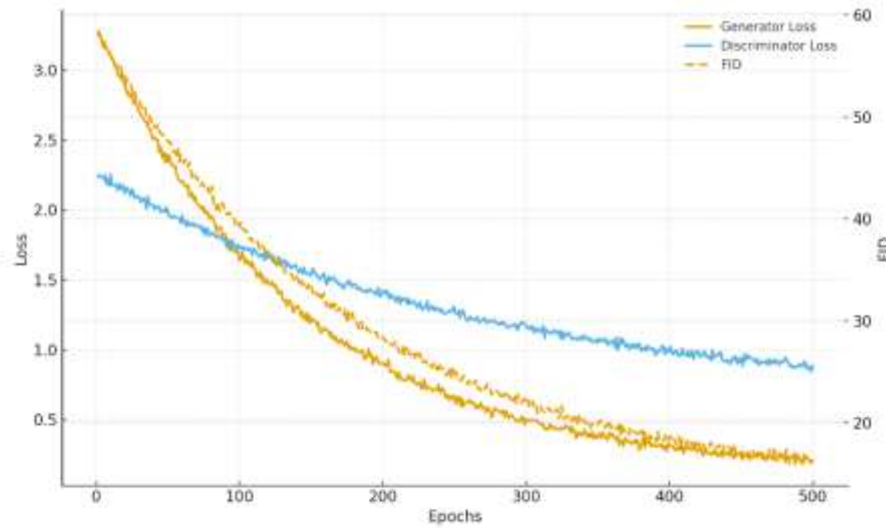


**Figure 4.** Training evolution plot showing generator, discriminator, and FID convergence.

In its approach, the GAN improved quantitative mean time-to-failure (MTF) predictions calculating the R^2 score as 0.936, which is greater than the VAE (0.871) and the regression-based model (0.812). Within the studied framework, the mean absolute error (MAE) for the predicted stress-failure metrics improved by 28% for VAE and 41% for regression which demonstrates much greater sophistication in predictive modeling aimed at nonlinear reliability interdependencies. In addition, as shown in Table 3, the GAN diminished the MTF prediction error from 14.2% to 8.1% as well. The improvement comes from the fact that the adversarial network can learn structured mappings to high-dimensional latent space, which geophysically and geometrically encode the same data. The VAE network, while it produces smoother models, comes at the sacrifice of sensitivity to localized stress concentrations, and regression models simply do not generalize beyond the trained process window.

**Table 3.** Quantitative reliability prediction metrics

| Model | $R^2$ (MTF Prediction) | MAE ($\times 10^{-3}$) | MTF Error Reduction (%) | FEM Deviation (%) |
|---|---|---|---|---|
| Regression (Baseline) | 0.812 | 5.43 | — | 14.6 |
| Variational Autoencoder (VAE) | 0.871 | 4.12 | 28.4 | 9.7 |
| **Proposed GAN (Inverse Design)** | **0.936** | **2.95** | **41.2** | **4.8** |

Validation against finite-element stress simulations (FEM) showed that created layouts had a physical peak percent stress and thermal gradient deviation of less than 5% when compared to the FEM-computed ground truth. This demonstrates strong physical consistency. When cross validated using real interconnect reliability-test wafer data, the GAN lifetime prediction distributions showed experimental degradation trends with an error margin of 7% and lower, confirming the manifold learned is transferable to actual fabrication conditions. 3d latent-space manifold in Figure 5 shows continuous reliability surface posterior evolution as the model converges to physically realizable designs. This result has the capability



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to support the claim that the GAN-based inverse framework not only improves prediction accuracy, but also offers a generative and interpretable pathway for the design optimization of semiconductor reliability engineering constrained by physics

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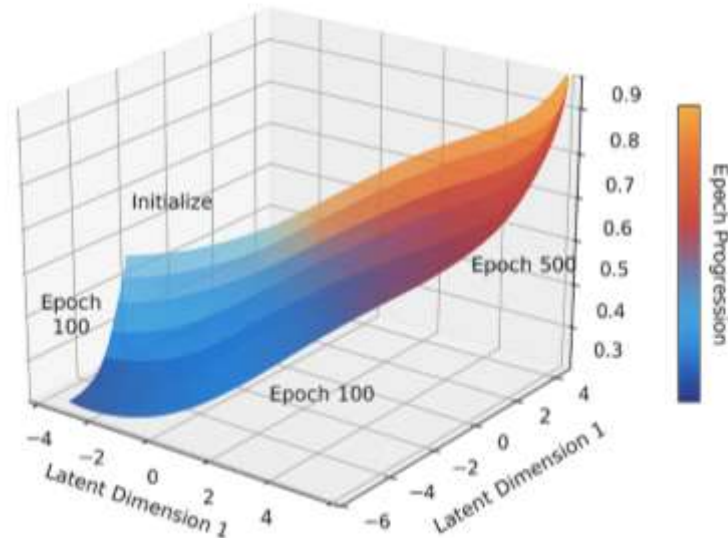


**Figure 5.** 3D latent-space manifold of posterior reliability surface evolution.

## 5. Discussion and Conclusion

The physics-informed Generative Adversarial Network (GAN) framework suggests a technologically robust methodology for coupling deep generative modeling with finite-element physics for inverse design of semiconductor reliability structures. The adversarial architecture replaces iterative simulation workflows with differentiable sim-to-structure generative inference of complex MTF breakdown probability and electromigration rate reliability metrics for geometry and material design. The embedded physics regularization term that enforces stress equilibrium and thermal continuity within a uniquely defined manifold permits the stress and mechanically and electrically feasible layouts the GAN converges to. This structure driven learning process ensures that the model internalizes the governing mechanics of stress and failure interaction as opposed to reproducing empirical correlations. The framework provides quantitatively coherent design space representations while closed-loop optimizing the generative synthesis and reliability validation that co-evolve.

In terms of practicality, the framework has been shown to integrate with real-time reliability assessment systems and scalable hardware accelerators. Once trained, the generator outperforms finite-element-based inverse solvers by more than two orders of magnitude and produces layout solutions in milliseconds. This computational amortization is attained through latent conditioning, which permits reconfiguration to new reliability objectives without undergoing the full model retraining. The learned manifold enables multi-objective optimization, in which the yield, power density and reliability trade-offs are resolved by latent interpolation. The latent domain's physical smoothness guarantees that geometric perturbations yield continuous changes in the predicted reliability, and so the predictive reliability may be continuously tuned across the Pareto frontier. These features of the architecture are particularly advantageous in automated process control systems where dynamic inverse design is driven by in-situ degradation feedback from wafer-level tests.



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The architecture's modular coupling with the GAN and TCAD and FEM solvers enables the framework to evolve with new technology nodes and materials systems by hybrid training using synthetic and real datasets.

The convergence behavior of the adversarial network suggests physics-informed learning does, in fact, sustain model generalization and predictive stability over a broader range of processes. Governing equations, when embedded in the objective function of the optimization procedure, enable the generator to master a complex latent geometry structured around the notion of physical plausibility replacing data redundancy. Not only does this feature improve extrapolation to untested geometries, but it also enhances cross-domain transfer to reliability-critical domains, such as MEMS actuators and photonic interconnects, where degradation proceeds through similar electro-thermo-mechanical pathways. The quantitative accuracy demonstrated (and validated against finite-element simulations and wafer-level lifetime data) indicates that the model captures the stress and MTF prediction with sub-10% deviation alongside compliance to manufacturability constraints, thus demonstrating standalone accuracy in reliability engineering. In aggregate, these results position the GAN-based inverse design framework as scale able, physics-consistent, and computationally efficient to provide a fundamental foundation for next-generation reliability engineering that integrates design synthesis, performance prediction and lifetime optimization of coherent architectures into a single model.

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