

AI-Assisted Microstructure Optimization of BaTiO₃ Ceramics for Ultrathin MLCC Applications

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Abstract

Multilayer ceramic capacitors have become foundational components in modern electronics, and their continued miniaturization depends on the precise control of barium titanate ceramic microstructures at thicknesses approaching the limits of conventional processing. This paper examines how artificial intelligence can assist the optimization of BaTiO₃ microstructures for ultrathin multilayer ceramic capacitor applications, with attention to system-level architecture, process integration, reliability governance, sustainability, and policy consequences. The discussion treats AI-assisted microstructure optimization not merely as a computational materials problem but as a socio-technical infrastructure that connects synthesis, tape casting, sintering, electrode integration, metrology, factory data systems, and regulatory expectations. The paper argues that the most consequential gains arise when machine learning models are embedded within closed-loop manufacturing and characterization environments rather than used as isolated predictive tools. It reviews microstructural constraints such as grain size, core-shell architecture, porosity, oxygen vacancy distribution, and dielectric breakdown, and it explains how surrogate models, Bayesian optimization, generative design, and physics-informed learning can support trade-off navigation across permittivity, loss, reliability, and yield. The paper also analyzes data infrastructure requirements, uncertainty management, distributional shift, model governance, and the risk of overfitting to narrow process windows. It considers sustainability and fairness implications, including energy intensity, critical materials, supply chain concentration, and equitable access to advanced manufacturing capabilities. Finally, it proposes a staged deployment roadmap that couples pilot-line validation, digital twins, human oversight, and standards development. The conclusion is that AI-assisted microstructure optimization can accelerate ultrathin MLCC development, but only if it is governed as an integrated materials and manufacturing system rather than as a narrow algorithmic intervention.

Keywords

AI-assisted materials design; BaTiO₃ ceramics; ultrathin MLCC; microstructure optimization; reliability; sustainable electronics; materials informatics; manufacturing governance.

1. Introduction

The modern electronics economy depends on passive components that are often invisible in public discourse yet essential to computation, communication, transportation, energy conversion, and medical devices. Among these components, multilayer ceramic capacitors occupy a central position because they provide high volumetric capacitance, low equivalent

series resistance, and compatibility with high-temperature assembly processes [1]. As electronic systems become more compact and power-dense, the demand for capacitors with thinner dielectric layers, higher capacitance per unit volume, and greater reliability under electrical, thermal, and mechanical stress has intensified [2]. Barium titanate, BaTiO_3 , remains the dominant dielectric material for high-performance multilayer ceramic capacitors because its perovskite structure supports high permittivity and because its properties can be tuned through doping, grain size control, and core-shell engineering [3]. However, the movement toward ultrathin layers exposes fundamental tensions between permittivity, breakdown strength, leakage current, aging behavior, and manufacturability. These tensions cannot be resolved by a single materials discovery step; they require coordinated optimization across powder synthesis, slurry formulation, tape casting, lamination, sintering, electrode formation, and final testing [4].

Artificial intelligence has entered materials science with the promise of accelerating discovery and reducing experimental burden. Machine learning models can identify complex relationships among composition, processing, microstructure, and properties that are difficult to capture with purely mechanistic models [10]. In the context of BaTiO_3 ceramics for ultrathin multilayer ceramic capacitors, the opportunity is substantial because the relevant design space is high-dimensional and the experimental cost of exploring it is high. Each variation in dopant chemistry, particle size distribution, binder system, sintering profile, atmosphere, and cooling rate can alter grain growth, core-shell formation, oxygen stoichiometry, and defect chemistry [5]. These microstructural features then influence dielectric constant, loss tangent, insulation resistance, and degradation under bias. An AI-assisted approach can help prioritize experiments, infer hidden process relationships, and support inverse design of microstructures that meet multiple performance targets simultaneously [11]. Yet the technical promise is only part of the story. The deployment of AI in ceramic capacitor manufacturing raises questions about data quality, model interpretability, factory infrastructure, workforce capability, reliability assurance, and the governance of automated decisions in safety-critical supply chains [18]. This paper therefore adopts a system-level perspective. It treats AI-assisted microstructure optimization as an integrated capability that must be designed, validated, governed, and sustained across technical and institutional boundaries.

2. Ultrathin MLCC Architecture and Microstructural Constraints

Ultrathin multilayer ceramic capacitors are not simply scaled-down versions of conventional devices. As dielectric layer thickness decreases, the electric field at operating voltage increases, and the consequences of microstructural heterogeneity become more severe. A pore, a coarse grain, a chemically inhomogeneous region, or a discontinuous electrode interface can become a locus of field enhancement, leakage, or breakdown [6]. The dielectric layer must therefore exhibit not only high permittivity but also uniform density, controlled grain size, minimized porosity, and stable defect chemistry. In BaTiO_3 , the ferroelectric-to-paraelectric transition near the Curie temperature creates a strong temperature dependence of permittivity, which is usually moderated by dopants that form core-shell structures. These core-shell architectures allow a relatively ferroelectric core to coexist with a more paraelectric shell, producing a broader and flatter capacitance-temperature response [7]. The optimization challenge is to achieve the desired core-shell morphology without introducing secondary phases, excessive grain growth, or oxygen vacancy concentrations that accelerate degradation.

Grain size is a particularly important control variable because it affects domain configuration, permittivity, and reliability. Early work on fine-grained barium titanate ceramics established that permittivity can exhibit a maximum at a critical grain size, after which further refinement may reduce permittivity while improving breakdown strength [8]. For ultrathin layers, the grain size must be small relative to the layer thickness to avoid local shorting paths and to maintain statistical reliability. However, very small grains can increase grain boundary density, alter dopant distribution, and introduce interfacial resistance that affects loss and capacitance stability. The sintering process must therefore balance densification against grain growth, a trade-off that becomes more difficult as layer thickness decreases. Aqueous tape casting has emerged as a promising route for producing high-performance BaTiO₃ films for ultrathin multilayer ceramic capacitor applications because it can reduce organic solvent burden and support environmentally preferable manufacturing, but it also places stringent demands on slurry rheology, binder burnout, and green sheet uniformity [9]. The interaction between tape casting chemistry and subsequent sintering means that microstructural optimization cannot be separated from upstream formulation and downstream thermal processing.

Electrode integration adds another layer of complexity. Base-metal electrodes such as nickel are widely used to reduce cost, but they require reducing atmospheres during sintering to prevent oxidation. These atmospheres can promote oxygen vacancies in BaTiO₃, which may migrate under electric fields and contribute to resistance degradation [5]. The dielectric composition, sintering atmosphere, cooling profile, and electrode chemistry must therefore be co-designed. In ultrathin devices, the interface between dielectric and electrode becomes a larger fraction of the total volume, so interfacial reactions, interdiffusion, and Schottky barriers have disproportionate effects. The capacitor is thus a coupled electrochemical and microstructural system, not merely a dielectric slab. AI-assisted optimization is valuable in this setting because it can model multivariate interactions that are difficult to isolate experimentally, but it must also respect the physical and chemical constraints that govern irreversible degradation.

3. AI-Assisted Microstructure Optimization Framework

An AI-assisted framework for BaTiO₃ microstructure optimization typically begins with data acquisition and representation. Data may come from historical production records, designed experiments, high-throughput synthesis, electron microscopy, X-ray diffraction, impedance spectroscopy, and electrical reliability testing. The quality and comparability of these data are often more important than the sophistication of the learning algorithm. Materials informatics has shown that curated datasets, standardized descriptors, and transparent provenance are essential for building models that generalize beyond the original laboratory conditions [10]. In the case of ceramic capacitors, relevant descriptors may include powder surface area, dopant concentration, binder chemistry, green density, sintering temperature, dwell time, atmosphere composition, cooling rate, grain size distribution, core-shell fraction, porosity, and electrode roughness. Because many of these variables are measured at different scales and with different uncertainty levels, the framework must include data fusion and uncertainty quantification rather than treating all inputs as equally reliable.

Supervised learning can be used to predict properties such as permittivity, loss tangent, insulation resistance, and breakdown voltage from processing and microstructural descriptors. However, simple regression models may fail when the process space is sparse or when the underlying physics changes across regimes. Physics-informed and hybrid models can improve

robustness by incorporating known constraints, such as densification kinetics, grain growth laws, or defect chemistry relationships [16]. Bayesian optimization is particularly appropriate for experimental campaigns because it balances exploration of uncertain regions with exploitation of promising compositions and process conditions [13]. Adaptive design methods have demonstrated that sequential decision-making can accelerate the search for materials with targeted properties, especially when each experiment is expensive and the property landscape is non-convex [14]. In ultrathin multilayer ceramic capacitor development, such methods could prioritize sintering profiles that maximize density while limiting grain growth, or dopant combinations that flatten temperature dependence without increasing leakage.

Generative models and inverse design introduce a different capability. Instead of predicting properties from a given microstructure, they propose microstructures or process routes that are likely to satisfy multiple objectives [15]. This is attractive for BaTiO₃ because the desired microstructure is often specified as a set of competing targets: high permittivity, low loss, high breakdown strength, stable capacitance with temperature, and long lifetime under bias. A generative model could, in principle, propose core-shell architectures, grain size distributions, or dopant gradients that are not present in the training data. Yet generative proposals must be constrained by thermodynamic feasibility, kinetic accessibility, and manufacturing compatibility. A microstructure that is theoretically optimal but cannot be produced reliably in a tape-casting and sintering line has limited industrial value. The AI framework must therefore be coupled to process simulation and experimental validation, not treated as a purely computational oracle.

The most mature architecture for AI-assisted optimization is a closed-loop system in which models, experiments, and manufacturing data interact continuously. In such a system, Bayesian optimization or reinforcement learning selects the next experiment or process adjustment, automated characterization provides feedback, and the model is updated. Over time, the system can learn local process sensitivities that differ among furnaces, tape casters, and electrode lines. This is important because ceramic manufacturing is subject to equipment-specific behavior, raw material variability, and environmental drift. A model trained in one facility may perform poorly in another unless it is adapted or recalibrated. The framework must therefore include transfer learning, domain adaptation, and uncertainty-aware decision policies [12]. The goal is not to replace ceramic engineers but to augment their ability to navigate a high-dimensional trade-off space with faster and more consistent feedback.

4. Process Integration, Sensing, and Data Infrastructure

The success of AI-assisted microstructure optimization depends on infrastructure that many materials laboratories do not possess. A factory or pilot line must be instrumented to capture process parameters, environmental conditions, material lot properties, and quality measurements at sufficient temporal and spatial resolution. Sensors for temperature, atmosphere, tape thickness, slurry viscosity, and electrode deposition must be calibrated and networked. Metrology tools such as scanning electron microscopy, impedance analyzers, and reliability test chambers must produce data in formats that can be linked to process history. Without this integration, AI models are limited to offline analysis of small historical datasets and cannot support real-time or near-real-time optimization [17]. The infrastructure challenge is therefore as much organizational as technical. It requires data governance policies, interoperability standards, cybersecurity controls, and a culture of documentation.

A digital twin of the capacitor manufacturing process can provide a unifying architecture. The digital twin represents the physical line, materials, and products in a computational

environment that is updated with sensor and test data. It can simulate the effect of proposed process changes, estimate uncertainty, and support scheduling of experiments. For ultrathin multilayer ceramic capacitors, a digital twin might combine slurry rheology models, tape casting simulations, sintering kinetics, microstructure evolution, and electrical property predictions. Machine learning can fill gaps where first-principles models are incomplete, while physical models can constrain predictions in regions where data are sparse. This hybrid approach is more robust than either pure simulation or pure data-driven modeling. It also provides a natural interface for human engineers, who can inspect assumptions, compare scenarios, and approve changes.

Data infrastructure must address the full lifecycle of models. This includes data acquisition, cleaning, versioning, feature engineering, model training, validation, deployment, monitoring, and retirement. In materials science, reproducibility is often compromised by inconsistent metadata and by the difficulty of capturing tacit process knowledge. AI systems can exacerbate this problem if they obscure provenance or if they produce recommendations that cannot be traced to specific data. Governance frameworks for artificial intelligence emphasize transparency, accountability, and risk management [18]. In a manufacturing setting, these principles translate into requirements for audit trails, model documentation, change control, and human oversight. The European approach to trustworthy artificial intelligence similarly stresses human agency, technical robustness, privacy, and societal well-being [19]. These frameworks are not merely bureaucratic additions; they are necessary for building confidence among customers, regulators, and supply chain partners.

5. Robustness, Reliability, and Failure Governance

Ultrathin multilayer ceramic capacitors are used in applications where failure can have serious consequences, including automotive electronics, medical devices, aerospace systems, and power infrastructure. An AI-assisted optimization system must therefore be designed for robustness under uncertainty. The operating environment of the model is not the same as the operating environment of the capacitor. The model may encounter new raw material suppliers, changed furnace conditions, aged equipment, or novel product designs. These shifts can invalidate learned relationships and lead to recommendations that appear statistically sound but are physically unsafe. Distributional shift is a central concern in machine learning for materials and manufacturing [13]. A model that predicts breakdown strength from grain size may fail when a new dopant changes the failure mechanism from bulk breakdown to interfacial degradation.

Reliability governance requires that AI recommendations be validated through accelerated life testing, voltage endurance tests, thermal cycling, humidity bias, and destructive physical analysis. Statistical reliability methods must account for the fact that failures in ultrathin dielectrics are often extreme-value phenomena. A small number of weak grains or pores can determine the lifetime of the entire device. Therefore, average property predictions are insufficient. The AI system should estimate tail risks, identify microstructural features associated with outliers, and flag conditions that require additional sampling. Uncertainty quantification is not an optional add-on; it is a core requirement for safe deployment. Ensemble methods, Bayesian neural networks, Gaussian processes, and conformal prediction can provide different forms of uncertainty estimates, but each has limitations. The choice of method should be tied to the decision context. For example, a process adjustment that affects millions of parts requires more conservative uncertainty treatment than an exploratory laboratory experiment.

Failure governance also involves human factors. Engineers may over-trust automated recommendations or, conversely, ignore them when they conflict with experience. The design of the human-machine interface matters. A useful system should show predicted outcomes, confidence intervals, contributing factors, and counterfactual explanations. It should allow engineers to impose hard constraints, such as maximum sintering temperature or minimum insulation resistance, and to document deviations. When a failure occurs, the system should support root-cause analysis by linking the failed part to its process history, characterization data, and model recommendations. This sociotechnical perspective aligns with risk management frameworks that treat AI as a component of a larger system rather than as an autonomous decision-maker [20]. The goal is not perfect prediction but resilient decision-making under uncertainty.

6. Sustainability, Fairness, and Policy Implications

The miniaturization of multilayer ceramic capacitors has environmental implications that are often overlooked. Thinner dielectric layers reduce material consumption per device, but the manufacturing process may require more energy-intensive sintering, tighter cleanroom conditions, and more complex quality control. Barium titanate production involves mining and processing barium and titanium precursors, while base-metal electrodes rely on nickel and other metals with their own supply chain impacts [2]. AI-assisted optimization can contribute to sustainability by reducing experimental waste, minimizing over-sintering, lowering scrap rates, and identifying compositions that require less critical material. However, it can also increase energy consumption if it encourages more extensive experimentation or more complex process control. The net sustainability effect depends on how the technology is deployed and governed. Life cycle assessment should be integrated into the optimization objectives rather than treated as an afterthought.

Fairness and equity are relevant in at least two ways. First, access to advanced AI-assisted manufacturing infrastructure is uneven. Large firms and well-funded research institutions may be able to build digital twins and closed-loop optimization systems, while smaller suppliers and institutions in lower-resource settings may be left behind. This could concentrate capacity and innovation in a few regions, reducing supply chain resilience and excluding diverse perspectives from materials design. Second, the data used to train models may reflect historical process windows and product priorities that do not represent the needs of all users. For example, automotive, consumer, and medical applications have different reliability requirements and different acceptable trade-offs. If models are trained primarily on high-volume consumer products, they may underperform for specialized or low-volume applications. Policy interventions could support open data standards, shared pilot facilities, and training programs that broaden participation in AI-enabled materials manufacturing [19]. Public procurement and research funding can also incentivize sustainability and reliability objectives.

Policy implications extend to standards, export controls, and liability. As AI systems become more involved in process decisions, questions arise about responsibility when a product fails. Is the manufacturer responsible, the model developer, the data provider, or the engineer who approved the recommendation? Clear documentation and audit trails are essential for assigning accountability. Standards bodies can help by defining requirements for data quality, model validation, and uncertainty communication in materials manufacturing. Risk management frameworks provide a starting point, but they must be adapted to the specific characteristics of ceramic processing, where physical mechanisms are complex and failure

may emerge only after long-term operation [20]. International cooperation may also be needed to avoid fragmented standards that increase costs and slow innovation. The governance challenge is to promote safety and trust without stifling the experimentation that makes AI-assisted materials design valuable.

7. Case Illustrations and Cross-Domain Comparisons

The development of ultrathin BaTiO₃ capacitors can be compared with other domains where AI has been used to navigate complex design spaces. In semiconductor manufacturing, machine learning is used for process control, yield prediction, and defect classification. The analogy is instructive because both domains involve multiscale physics, expensive experiments, and stringent reliability requirements. However, ceramic capacitors differ in that their microstructure evolves through sintering and is not directly patterned like a semiconductor circuit. The relevant data are often image-based, three-dimensional, and noisy, which makes representation learning both promising and difficult [11]. In battery materials, AI has been used to discover new electrolytes and electrode compositions by combining high-throughput experiments with active learning [14]. That experience shows that data infrastructure and experimental automation are often the limiting factors, not the algorithms themselves.

In pharmaceutical development, AI-assisted formulation has demonstrated the value of surrogate models and Bayesian optimization for navigating regulatory and stability constraints [13]. The comparison highlights the importance of validation and documentation. A formulation recommendation that works in a laboratory may fail in scale-up or in long-term storage. Similarly, a microstructure recommendation for BaTiO₃ may succeed in a small tape-cast sample but fail in a multilayer stack with electrodes and high-field operation. Cross-domain learning suggests that the most successful deployments are those that embed AI within an experimental and regulatory workflow rather than presenting it as a standalone prediction engine. Generative design in molecular and materials science also offers lessons about the need for synthesizability and processability constraints [15]. A generated microstructure must be manufacturable, and a generated process route must be compatible with existing equipment and safety requirements.

8. Deployment Roadmap and Future Perspectives

A realistic deployment roadmap for AI-assisted microstructure optimization in ultrathin multilayer ceramic capacitor manufacturing should be staged. In the first stage, historical data are curated and used to build predictive models for specific unit operations, such as tape casting thickness or sintering density. These models are validated against designed experiments and used to support human decision-making. In the second stage, models are integrated into a digital twin that links multiple process steps and enables scenario analysis. At this stage, uncertainty quantification and data governance become central. In the third stage, closed-loop optimization is introduced in a pilot line, with human approval required for process changes. In the fourth stage, select decisions may be automated within bounded operating windows, but only after extensive reliability validation and regulatory review. This staged approach reduces risk and allows organizations to build trust incrementally [18].

Future research should focus on several directions. One is the development of physics-informed machine learning that can combine continuum models of sintering and dielectric breakdown with data-driven corrections. Another is the creation of standardized microstructure descriptors and benchmark datasets that allow models to be compared across

laboratories. A third is the integration of sustainability metrics into multi-objective optimization, so that energy use, material criticality, and end-of-life recovery are considered alongside electrical performance [17]. A fourth is the study of human-AI collaboration in materials engineering, including how engineers interpret uncertainty and how organizational incentives shape the adoption of AI recommendations. Finally, policy research should examine how standards, liability rules, and public investment can support trustworthy and equitable deployment [19]. The technical and social dimensions are intertwined. A model that is accurate but not trusted, or efficient but not sustainable, will not achieve its full potential.

9. Conclusion

AI-assisted microstructure optimization offers a powerful approach to the development of BaTiO₃ ceramics for ultrathin multilayer ceramic capacitors. The core technical opportunity lies in using data-driven and physics-informed models to navigate the complex relationships among composition, processing, microstructure, and electrical reliability. Bayesian optimization, surrogate modeling, generative design, and digital twins can help engineers explore a high-dimensional design space with fewer experiments and better trade-off awareness. However, the most important challenges are systemic. Ultrathin multilayer ceramic capacitors are manufactured through coupled process steps, characterized by multiscale metrology, and deployed in safety-critical applications. AI systems must therefore be integrated with process infrastructure, validated under distributional shift, governed with transparent uncertainty, and aligned with sustainability and fairness goals. The required transformation is not simply algorithmic but organizational and institutional. It involves data standards, pilot-line instrumentation, workforce development, reliability science, and policy frameworks that clarify responsibility and build trust. If these conditions are met, AI-assisted microstructure optimization can accelerate the next generation of ultrathin multilayer ceramic capacitors while improving consistency, reducing waste, and expanding the range of achievable performance. If they are neglected, the result may be fragile models and fragmented adoption that fail to deliver on the promise of intelligent materials manufacturing.

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