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# Simulating the Co-Evolution of Porous Microstructures and Grain Growth in Sintered Ag Die Attach Layers

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**Abstract**

In this study, we introduced a hybrid Potts-phase field model to simulate the co-evolution of grain growth and pores migration in sintered silver layers. The Potts model is good at capture the grain growth dynamics, while the phase field model describes the evolution of the porous network. These models are coupled via a hybrid free energy function to achieve a realistic representation of the microstructure evolution. This study further extends the hybrid model by incorporating (a) a flexible exchange interaction matrix to model the crystal anisotropy in grain growth, (b) Glauber or Kawasaki dynamics to describe different diffusion mechanisms, and (c) the effect of pinning sites, representing impurity-driven grain boundary stabilization. The computational framework is implemented using Taichi Lang, which allows for efficient parallel simulations. Results show that the model effectively captures the long-term evolution of the sintered silver microstructure in good agreement with experimental observations. This hybrid model is a powerful tool to predict microstructural reliability of sintered silver die attach layers, supporting material design and process optimization for high-power electronic applications.

## 1. Introduction

Micro-nanoscale metal sintering materials, especially Silver (Ag) sintering materials, are extensively utilized as die-attach solutions in high-power device packaging due to their low-temperature sintering capabilities and excellent thermal and electrical conductivities [1–3]. Normally, Ag sintering materials are composed of micro/nano-sized particles, allowing particles to be sintered at low temperatures (150 - 300 $^{o}$C) below the melting point of bulk Ag (961 $^{o}$C) to build a porous microstructure. However, during continuous high-temperature and high-power operation, microstructure changes of the sintered Ag copper layer may affect the long-term reliability of the die-attach layer in high-power devices. Previous studies have investigated the degradation behaviors of sintered Ag layers under high-temperature storage (HTS), thermal cycling (TC), and TS, such as porosity evolution, interfacial oxidation, and mechanical property degradation [4–9].

Studying the evolution of material microstructure evolution, such as defect structure, grain size, composition distribution, etc., is crucial for understanding and predicting its mechanical, electrical, and thermal properties. Although characterization techniques such as scanning electron microscopy (SEM) and electron backscatter diffraction (EBSD) can provide insights into microstructural evolution, their high cost, time consumption, and limited resolution at the micro- and nanoscale make their effectiveness in predicting the long-term aging behavior of materials challenging [5, 8].

From the simulation perspective, grain growth and pore evolution are typically simulated independently. At the atomic scale, Molecular Dynamics (MD) tracks the motion trajectory of each atom based on Newton's equation of motion, but the time and space scales are different from actual conditions [10]. At the mesoscopic scale, the Kinetic Monte Carlo (KMC) method, such as the Q-state Potts model[11–13], provides an efficient way to simulate grain growth while capturing stochastic diffusion processes over long timescales. However, it neglects complex effects such as elasticity and stress. The phase-field method, based on continuous field variables, effectively describes interface evolution and pore morphology changes, offering better alignment with real-world spatial and temporal scales [14, 15]. Although versatile and flexible, phase-field modeling is mathematically complex and computationally demanding [16–18]. The macroscopic finite element method considers the influence of the stress field and temperature field on microstructure but is not good at interface tracking [19]. Other microstructural evolution methods, such as cellular automata, level set methods, and hybrid phase-field approaches, have also been explored [20–23]. At present, there is still a lack of simulation methods for the co-evolution of pores and grain structures in complex microstructures on a long-term scale to predict the microstructure and reliability of materials during service.

In this work, we present a hybrid Potts–Phase field model to simulate the co-evolution of porous microstructure and grain growth in the bonding layer of sintered Ag chips. The Potts model is employed to discretely represent lattice states, while the phase-field model con-

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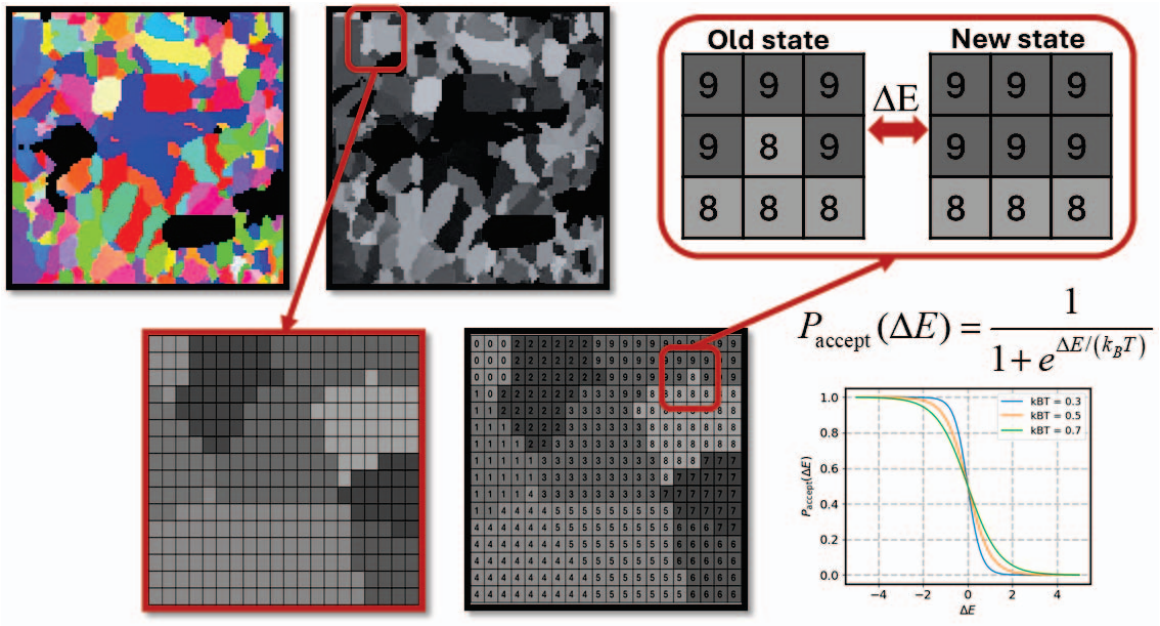


Figure 1. Schematic diagram of lattice evolution in Potts model, including Monte Carlo step update process and acceptance probability.

tinuously describes the evolution of composition fields. These models are coupled through a hybrid free energy function to achieve a more comprehensive representation of microstructural changes. This work is written in Taichi Lang, a programming language embedded in Python, to achieve high-performance parallel computing. To extend the capabilities of the classic hybrid Potts-Phase field model, we introduce several enhancements: a. A flexible exchange interaction energy matrix to account for grain growth dominance along specific crystallographic orientations. b. Both Kawasaki and Glauber dynamics describe grain diffusion and rearrangement processes. c. Pinning sites that remain static during evolution represent the effects of impurity distributions on microstructural development. These advancements enable a more realistic and predictive framework for studying the long-term evolution of sintered Ag microstructures under high-temperature operating conditions.

## 2. Theoretical Background

### *A. Hybrid Potts-Phase Field Model*

The Potts model, an extension of the Ising model, serves as a robust framework for simulating microstructural evolution in polycrystalline materials. A schematic diagram of the simulation mechanics is provided in Figure 1. In this model, the microstructure is discretized into a regular lattice grid, where each lattice site represents a grain state, denoted as $q_i$. The total energy of the system is defined as:

$$E_{\text{Potts}} = \sum_{\langle i,j \rangle} J_{q_i,q_j} \left(1 - \delta_{\sigma_{q_i},\sigma_{q_j}}\right) \tag{1}$$

Here, $J_{q_i,q_j}$ represents the interaction energy between neighboring grain states, and $\delta_{\sigma_{q_i},\sigma_{q_j}}$ is the Kronecker delta, equaling 1 when $q_i = q_j$ (indicating sites within the same grain) and 0 otherwise (indicating a grain boundary). To simulate abnormal grain growth (AGG), the interaction energy matrix $J_{q_i,q_j}$ can be selectively modified to favor the preferential growth of specific grains, such as by assigning lower boundary energies to certain grains, thereby accelerating their expansion. Conversely, for normal grain growth (NGG), the matrix $J_{q_i,q_j}$ is set to reflect uniform interaction energies across all grains, promoting a homogeneous growth pattern. Figure 2 compared Normal and Abnormal grain growth simulation by Potts model.

The evolution of the system is governed by the Metropolis algorithm, a Monte Carlo method that captures the stochastic dynamics of grain boundary migration. At each simulation step, a randomly selected lattice site attempts to change its state (i.e., its grain orientation). The energy difference $\Delta E$ resulting from this proposed change is calculated, and the acceptance of the new state is determined using the Boltzmann probability:

$$P_{\text{accept}} = \frac{1}{1+\exp(\Delta E/k_B T)} \tag{2}$$

where $k_B$ is the Boltzmann constant and $T$ is the system temperature. This probabilistic rule accounts for thermally activated processes, with the temperature parameter $T$ playing a critical role in regulating the likelihood of overcoming energy barriers. A higher temperature increases the acceptance probability of energetically unfavorable changes, introducing greater randomness, while a lower temperature favors energy minimization, leading to more deterministic grain boundary migration.

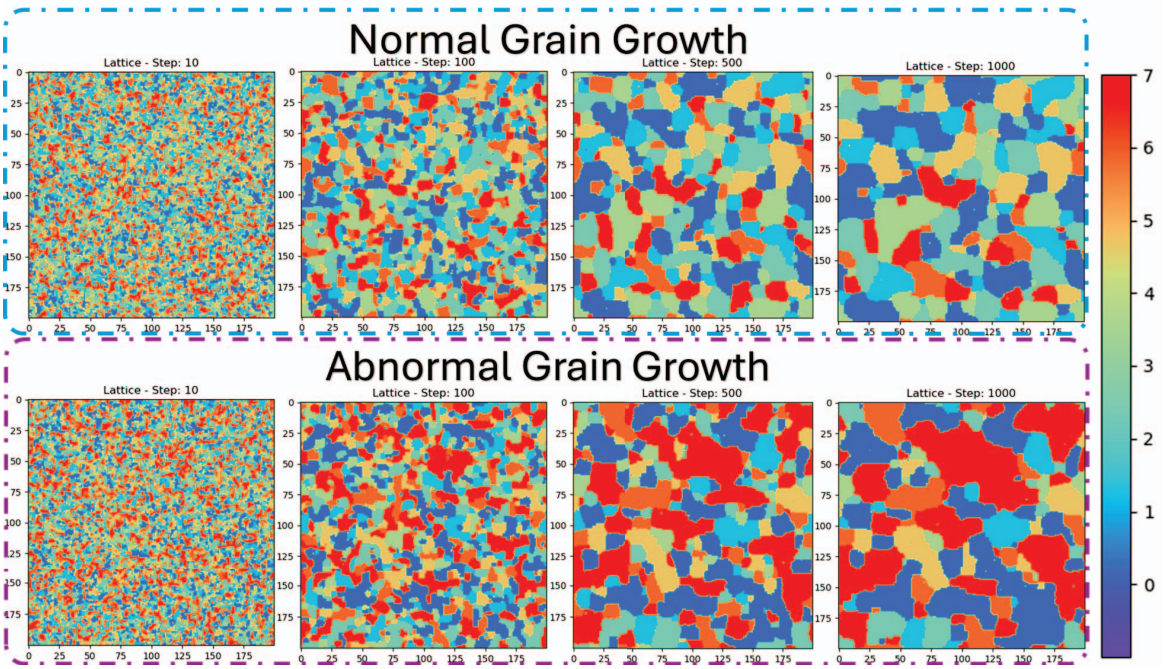


Figure 2. Comparative evolution of normal vs. abnormal grain growth in the Potts model.

In addition to the discrete phase states $q_{ij}$, each grid point also defines a composition field represented by a continuous order parameter $C_{ij}(x,t)$. The system evolution is governed by the Cahn-Hilliard equation:

$$\frac{\partial C}{\partial t} = M_c \left\{ \nabla^2 \frac{\partial E_v}{\partial C} - \kappa_C \nabla^4 C \right\} \tag{3}$$

where $M_c$ is the mobility that controls the evolution speed and $\kappa_c$ is the composition field gradient energy coefficient. $E_v$ is the volume free energy. To describe the two-phase (in this case, Ag and pore) separation evolution process, the form of $E_v$ is

$$\begin{aligned} E_v(C_{ij}, q_{ij}) &= k\left[(C_{ij} - C_1)^2 + (C_2 - C_{ij})^2\right] \\ &= +a\left[(C_{ij} - C_3)^2 q_a + (C_4 - C_{ij})^2 q_b\right] \end{aligned} \tag{4}$$

Here, $C_{ij}$ is the composition field, $q_{ij}$ represents the lattice state, and $q_a$ and $q_b$ indicate Phase A and Phase B, respectively. Parameters $C_1$ and $C_2$ define the baseline double-well potential, while $C_3$ and $C_4$ set preferred compositions for Phases A and B. Coefficients $k$ and $a$ control the strength of the double-well and phase-dependent terms, respectively, enabling phase separation and coupling between $C_{ij}$ and $q_{ij}$. The effects of varying these parameters on $E_v$ are illustrated in Figure 3, which demonstrates how changes in $k$, $a$, $C_1$, $C_2$, $C_3$ and $C_4$ influence the energy landscape across the composition range.

The hybrid Potts-Phase field model combines the advantages of the discrete Potts model to simply and efficiently control the non-conservative grain evolution and the phase field to more accurately capture the continuous component field evolution process. The total system energy in the hybrid model integrates both discrete and continuous components:

$$E_{\text{hybrid}} = \sum_{i=1}^{N} \left( E_v(q_i, C_i) + \sum_{j=1}^{n} J(q_i, q_j) + \kappa_c (\nabla C_i)^2 \right) \tag{5}$$

For a Monte Carlo step (Δt, where the actual time scale of Δt is not explicitly defined in this work) in the hybrid model, a grid point is randomly selected and its state is tried to be changed, such as changing q=8 in Figure 1 to q=9, and the local energy difference ΔE caused by this state change is calculated. This energy difference includes the interaction energy difference in the Potts model and the free energy difference caused by the change of the component field in the phase field model. The calculation of the interaction energy takes into account the eight-neighborhood relationship, and the evolution of the component field is updated using the explicit finite difference method according to the Cahn-Hilliard equation. Then, the probability $P_{accept}$ is used to decide whether to accept this change, so that the system evolves in the direction of lower energy.

### *B. High-performance Parallel Computing with Taichi Lang*

Taichi is an open source, high-performance programming language designed for numerical computation and physical simulation. [24] Since both the Pott model and the phase field model require large computing resources, this work was written in Taichi to efficiently handle complex data structures.

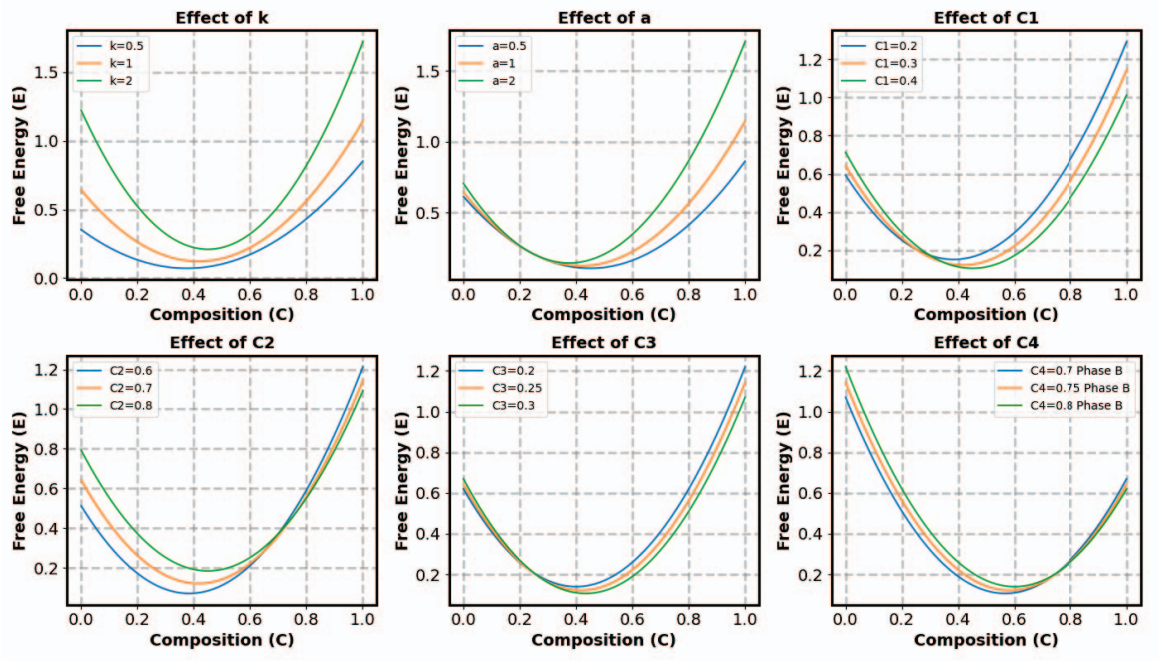


Figure 3. Effects of Parameters on Volumetric Free Energy $E_v$ as a function of Composition $C$. Each subplot shows the impact of varying a single parameter $k$, $a$, $C_1$, $C_2$, $C_3$ and $C_4$ on the energy landscape, highlighting their roles in shaping phase preferences.

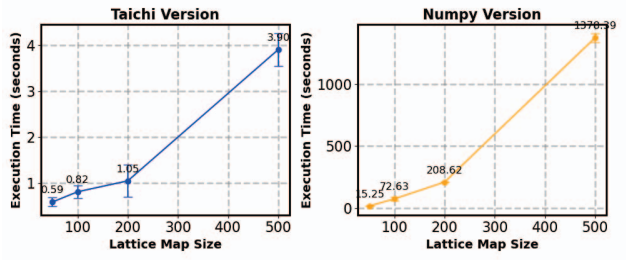


Figure 4. Execution time with differents map sizes: Taichi vs. Numpy.

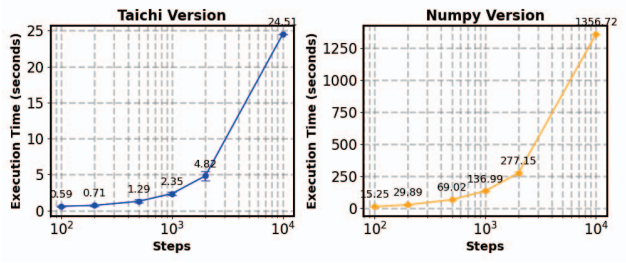


Figure 5. Execution time with differents steps: Taichi vs. Numpy.

Figure 4 presents the execution time (in seconds) for different lattice map sizes between Taichi and Numpy. The x-axis represents the lattice map size (number of grid points contained in the edge length), while the y-axis represents the execution time in seconds. As the lattice size increases, both implementations show an increase in execution time. However, the growth rate is much steeper for Numpy than for Taichi. For a 500 X 500 lattice, the Taichi version runs in about 3.9 seconds, whereas the Numpy version takes over 1376 seconds.

Figure 5 compares the execution time for different numbers of simulation steps between Taichi and Numpy. The x-axis represents the number of Monte Carlo steps (logarithmic scale), while the y-axis represents the execution time in seconds. The Taichi version shows a much lower execution time compared to the Numpy version, especially as the number of steps increases. The execution time for Taichi remains below 25 seconds even for 10,000 steps, while Numpy takes more than 1350 seconds for the same number of steps. The scalability of Taichi is significantly better, demonstrating its efficiency in handling large-scale simulations.

## 3. Simulation Results and Discussion

### *A. Initial Lattice Map, Composition Map, and Phase Field Map*

There are two forms of lattice map initialization. One is random state assignment, which randomly assigns states to sites according to the defined number of states. The other is image-based assignment, where each pixel is regarded as a site and different state values are assigned to the sites according to the grayscale value. After the Lattice map is initialized, the Phase map can be divided according to the state. For example, the state $q = 0$ is defined as pores, and the other states $q = 1, 2, 3, .., 7$ are defined as Ag in different crystal orientations. The Composition map is further assigned according to the Phase map. For the pore phase, the $C_{ij}$ value ranges from 0 to 0.5, and the $C_{ij}$ value ranges from 0.5 to 1 for the Ag phase.

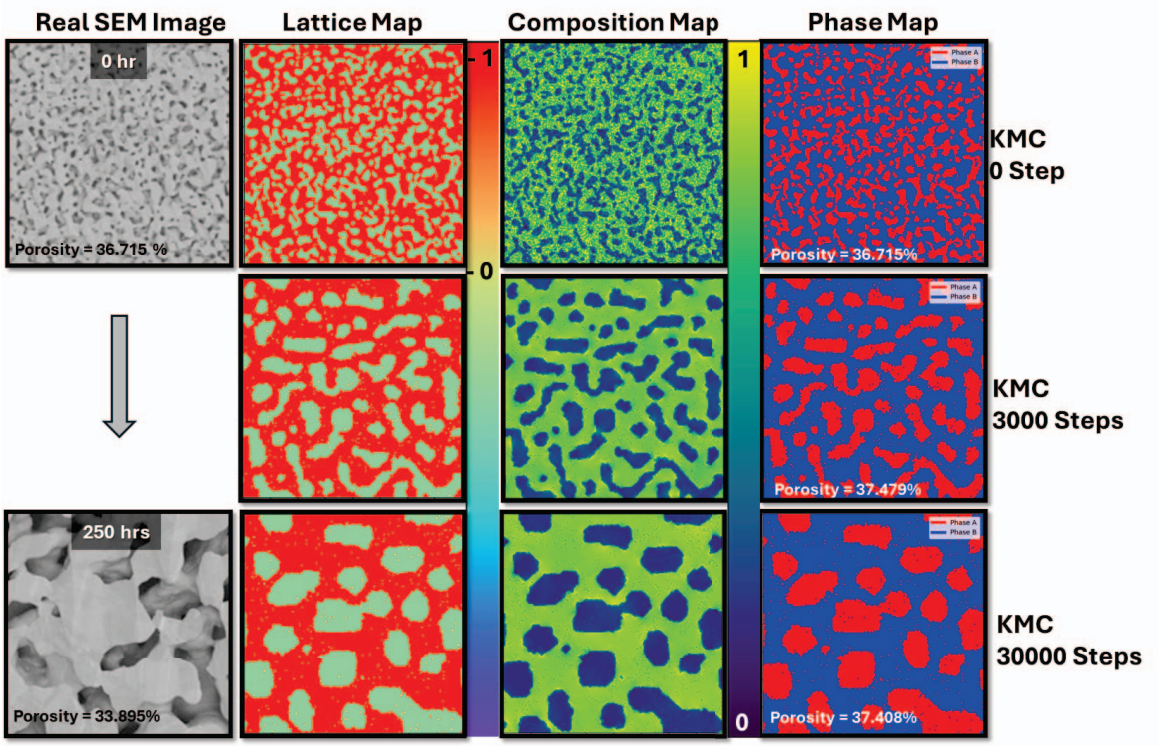


Figure 6. Microstructural evolution under Kawasaki dynamics.

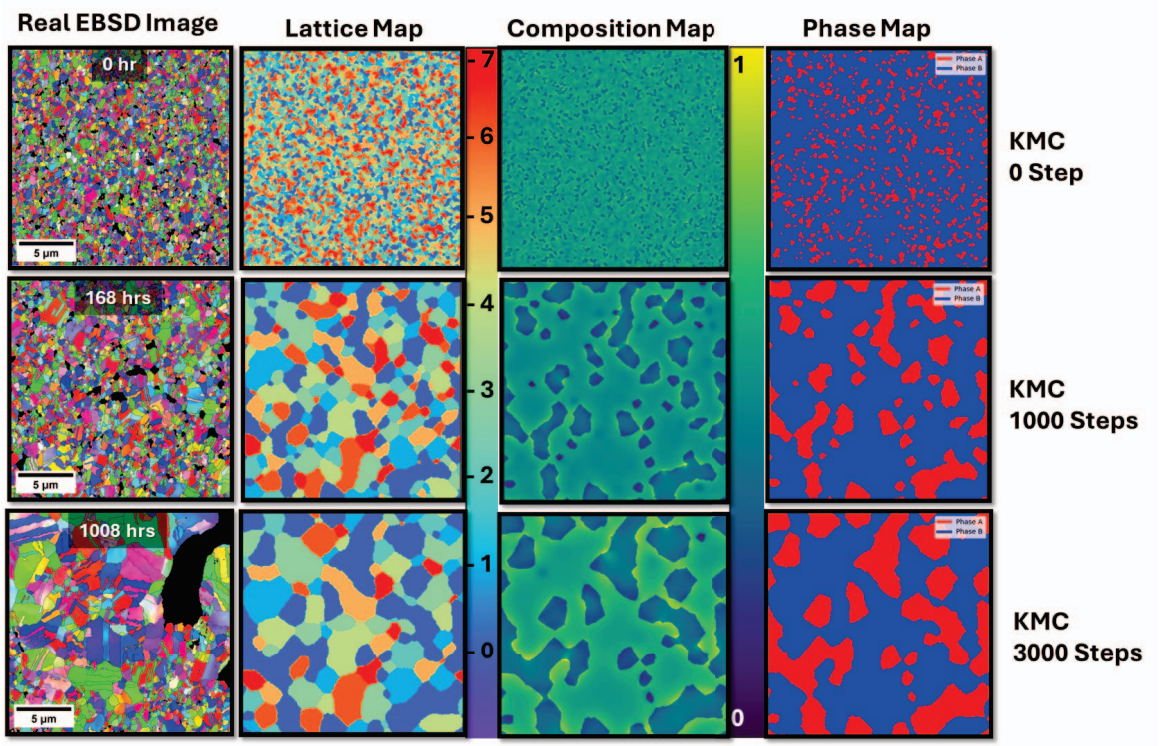


Figure 7. Microstructural evolution under Glauber dynamics.

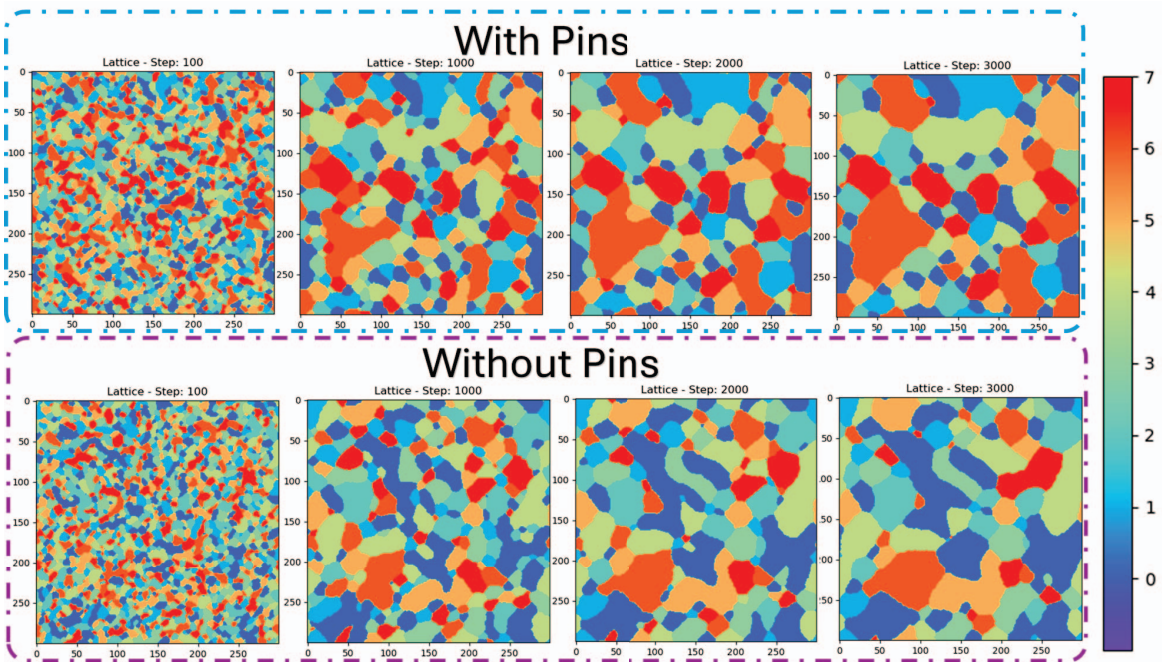


Figure 8. Effect of pins on grain growth and pore migration in the hybrid model.

### B. Microstructure Evolution Simulation

There are two different dynamics commonly used in Potts model simulations, Glauber dynamics and Kawasaki dynamics. Glauber dynamics involves site-based turnover, where individual sites randomly select new states, making it well suited for simulating grain growth and phase transitions in non-conservative systems. In contrast, Kawasaki dynamics forces state exchange between neighboring sites while maintaining the conservation of the total state distribution, making it more suitable for simulating diffusion processes in conservative systems, such as multi-component phase separation.

*1) Pore Migration Simulation - Kawasaki Dynamic:* Figure 6 shows the microstructural evolution of the Kawasaki dynamics simulation, which preserves the total phase fraction by forcing the exchange of states between adjacent sites rather than allowing independent state flips. This approach is well suited to simulating phase separation in conservative systems, and the pore migration in Ag sintering materials is described here. The left column shows experimental SEM images of sintered Ag at different aging times (0 hours and 250 hours). The lattice map was initialized based on the SEM image on the left. The pores are small and randomly distributed uniformly at the beginning, and irregular large pores are formed after 250 hours. The middle two columns show the changes in the distribution of Ag and pores in the Lattice map and Composition map. The right column shows the binary phase map, distinguishing between pores (red, phase A) and Ag (blue, phase B). The Kawasaki dynamics simulation successfully captures the coarsening of pores over time while maintaining overall phase conservation. The experimental and simulation results show similar trends in the evolution of porosity and pore morphology.

*2) Grain Growth and Pore Migration Simulation - Glauber Dynamic:* Figure 7 illustrates Glauber dynamics, a non-conserved stochastic update mechanism that allows individual lattice sites to change state freely, making it well-suited for simulating grain growth and coarsening. The left column presents experimental EBSD maps at different aging times (0 hr, 168 hrs, and 1008 hrs), revealing grain coarsening over time. The middle columns depict simulation results using Glauber dynamics, showing how grain structures evolve under Monte Carlo steps. The right column visualizes the simulated phase evolution with a binary representation of different phases. The Glauber dynamics simulation captures grain coarsening, where small grains disappear and larger grains grow over time. The simulation results closely match the experimental trends, confirming that Glauber dynamics effectively models grain growth.

### C. Effect of Pins

In the hybrid model, we introduce Pins sites to describe the influence of pinning effect on microstructural evolution. Pin sites do not change state during the simulation process, just like impurities at fixed positions. Figure 8 compares the evolution of grain growth and pore migration under different conditions—with and without pins—over multiple Monte Carlo steps (100, 1000, 2000, and 3000). The top row represents the case with pins, while the bottom row represents the case without pins. Different colors represent different grains. There are 8 states here,

q=0 is pores, and other q values represent Ag. The lattice size is 300 × 300, and the number of pin sites is 1000, accounting for approximately 1.1% of the total lattice sites.

The presence of pins (typically second-phase particles or obstacles) significantly impedes grain boundary motion, leading to localized pinning effects. As a result, some grains become anchored, preventing them from freely merging with neighboring grains. This restriction slows down grain coarsening compared to the case without pins. Additionally, smaller grains persist longer, demonstrating the resistance of pinning to grain growth. In contrast, when no pins are present, grains coarsen rapidly, merging into larger grains within the Monte Carlo steps. Pores migrate and coalesce, forming larger and more continuous voids. The resulting grain size distribution is more uniform compared to the pinned case, where grain boundary motion is inhibited. These results emphasizes the key role of pinning in microstructural evolution, which is important for material design to control grain size and improve mechanical properties.

## 4. Conclusions

This study introduces a Hybrid Potts-Phase Field Model to simulate the co-evolution of grain growth and pore migration in sintered Ag die-attach layers under high-temperature operating conditions. By integrating the discrete grain growth mechanism of the Potts model with the continuous phase evolution of the Phase-Field method, this model overcomes limitations of conventional simulation techniques and provides a comprehensive representation of microstructural changes. The key findings are summarized as follows:

- **Co-Evolution of Porous Microstructures and Grain Growth:** The hybrid model combines the characteristics of the Potts model, which is good at capturing grain coarsening and normal/abnormal grain growth, and the phase field model, which is effective in describing pore migration and coalescence, so that it can track the microstructural evolution of pores and grain growth during long-term aging, and is verified by experimental EBSD and SEM observations.
- **Different Evolution Mechanisms:** Glauber dynamics enables site-based flipping updates, making it suitable for simulating non-conserved grain growth and coarsening. Kawasaki dynamics enforces state conservation, making it well-suited for pore migration and phase separation simulations in sintered Ag materials.
- **Effect of Pinning Sites on Grain Coarsening:** The introduction of pinning sites leads to localized grain boundary stabilization and suppression of grain coarsening. Pinning effects significantly alter the final grain size distribution, leading to a more stable microstructure. Compared to simulations without pinning, grain growth is slowed down, and smaller grains persist longer.
- **Computational Performance and Efficiency:** The model is implemented in Taichi Lang, a high-performance computational framework optimized for parallel processing. Benchmarking against Numpy-based implementations shows that Taichi achieves substantially higher computational efficiency, making this model scalable for large-scale simulations.

Future work will focus on further parameter optimization for improved agreement with experimental data, extending the model to incorporate mechanical stress effects, and integrating multi-physics simulations to explore the interaction between microstructure evolution and thermal-mechanical reliability of sintered Ag die-attach layers in high-power applications.

## 5. Acknowledgements

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