

# In situ Electron Tomography-driven Bayesian Data Assimilation for High-fidelity Phase-field Simulation of Solid-state Sintering

Phase field (PF) simulation has emerged as a promising tool for predicting microstructural evolution during solid state sintering, offering a continuum framework that can capture neck growth, grain growth, and densification at the nano- and mesoscales. However, PF simulations demand accurate material parameters—such as temperature-dependent diffusion coefficients, interfacial energies, and mobilities—that are often unknown or difficult to obtain experimentally, limiting their quantitative reliability. To overcome this limitation, we developed a Bayesian data assimilation (DA) workflow that integrates in situ electron tomography/scanning transmission electron microscopy (STEM) observations into a PF simulation of copper nanoparticle sintering. Using a non-sequential assimilation scheme named DMC-TPE, the time-series of 3D particle morphologies was used to inversely estimate seven material parameters. The calibrated PF model reproduced the experimentally observed neck growth and densification with high-fidelity. This approach established a practical workflow for constructing digital twins of solid-state sintering processes, bridging in situ microscopy and physics-based simulation. We demonstrated that even limited in situ datasets can improve model reliability, offering experimentalists a powerful tool to interpret and guide sintering experiments. This work was supported by JST CREST (JPMJCR18J4).

## Professional Status of the Speaker

Senior Scientist

## Interest in submitting a paper in a special issue of

No interest

## Invitation letter for visa

No

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