ELECTROCHEMICAL-MECHANICAL PHASE FIELD MODEL FOR ELECTROPLATING PROCESS

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In order to prevent corrosion, electroplating is widely used in industrial processes. However, current practices for optimizing the electroplating process heavily rely on experimental efforts which are often very time consuming and labor intensive. In addition, it is difficult to quantify and optimize coating performance due to inherent uncertainties and the presence of many processing variabilities. Here, we propose a new electrochemical-mechanical phase field model associated with molecular dynamics approach. The proposed model involves all the complexities in the electroplating process, such as mass transport, reaction kinetics, interfacial anisotropy and the variations of electric and stress fields. By employing a generalized Butler-Volmer equation to describe the electrodeposition kinetics and expressing the free energy of the system as the sum of chemical potential, interfacial energy, electrostatic potential energy, and mechanical strain energy, the PF model captures the underlying physics of the electroplating process, particularly related to the coupling of the electrodeposition kinetics with specific mechanical properties. This study provides a strategy for optimizing electroplating process guided by a multiscale model integrating the phase-field method and atomistic calculations.

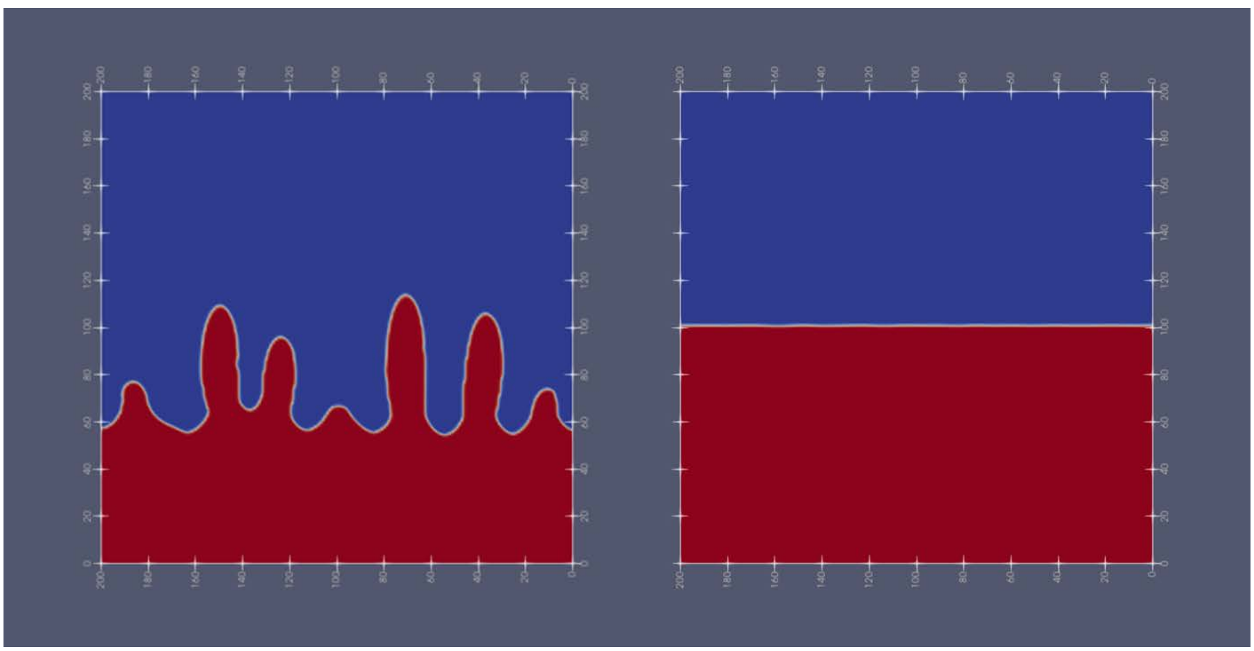

Figure 1 – Surface diffusion effect on morphology evolution