Machine learning approach of surface elastic chemical potential for morphological evolution of strained films

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The implementation of Deep learning for simulating surface dynamics during deposition emerges as a trustworthy and efficient tool to support and anticipate costly experiments. In strained thin films, the calculation of elastic energy term demands resorting to computationally intensive approaches, which remains the bottleneck when dealing with time evolutions. In this work, we explored the possibility of by-passing the explicit solution of the elastic problem by using a convolutional Neural Network (NN) to immediately predict the μ_ϵ profile associated to any surface profile. To this goal, we trained a NN on a dataset, composed of surface profiles and associated μ_ϵ, and showed that the NN reported an accurate prediction of μ_ϵ associated to any arbitrary surface geometry. Then, the NN is applied to the time integration of morphological evolutions in strained thin films, as shown by the performance of some cases (e.g. island growth and coarsening including substrate wetting effects), in which accuracy and numerical robustness are proven on large domains and long times. First, we use a dataset where $\mu\varepsilon$ is computed based on a Green's function approximation. In light of using a more accurate and quantitative solution, the same approach has been tested on a training set based on Finite Element Method (FEM) calculations of the elastic field. In this case, NN predictions reported the same accuracy as conventional numerical methods and, more notably, a 10^4 computational speed-up was achieved against FEM solver, which would allow to replicate scenarios that would otherwise be unfeasible. The proposed method could be extended or modified to include more complex phenomena (e.g. anisotropic surface energy density or the presence of plasticity-related objects such as dislocations).