Modeling growth of epitaxial nanostructures by continuum methods and machine learning.

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Both the typical timescale and sizes involved in epitaxial growth are a major challenge when attempting to simulate the process at the atomic scale. Therefore, continuum approaches have been developed allowing one to match experimental conditions. Despite yielding only an average description of the system behavior, continuum models can tackle several realistic aspects of growth such as preferential exposure of crystalline facets, strain relaxation, and out of equilibrium morphologies [1]. Examples of all such complexity will be given by analyzing our results on several diverse systems such as films, pillars, islands, and nanowires.
While working at the continuum level allows for a significant reduction of the computational costs, there is still the need of further speeding up simulations, particularly when use of finite element methods is required at every timestep. We shall show that a convenient convolutional, recurrent neural network approach [2] can tackle the problem of predicting structural evolution by surface diffusion, after being trained on a phase-field generated dataset. While showing good accuracy, the ML approach guarantees very significant speed ups.
Exciting perspectives, also in terms of extending machine-learning approaches beyond deterministic models, are discussed.

References

[1] Albani, M et al., "Faceting of Si and Ge crystals grown on deeply patterned Si substrates in the kinetic regime: phase-field modelling and experiments", Sci. Rep. 11, 18825 (2021).
[2] Lanzoni, D et al., "Morphological evolution via surface diffusion learned by convolutional, recurrent neural networks: Extrapolation and prediction uncertainty", Phys. Rev. Mat. 6, 103801 (2022).