Machine-Learning enabled acceleration of growth simulations

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Simulating the morphological evolution of thin films and nanostructures during deposition has always been a challenge due to the extremely long time scales involved. Experiments, indeed, span typical human scales of seconds or more, while time steps in atomistic molecular dynamics (MD) simulations must be of the order of femtoseconds. Kinetic Monte Carlo (KMC) approaches and, most importantly, continuum models (CMs) can help closing the gap between theory and experiments, as pictorially illustrated in Fig. 1. But if realistic CMs including e.g. preferential facet exposure, anisotropic growth kinetics, or mismatch strain are needed, then even such approaches necessitate for a further acceleration. In the last few years the "Machine Learning (ML) revolution" influenced all scientific sectors (and several non-scientific as well), including growth modeling. Here we shall briefly describe some advancements obtained in our group in this field (for a recente review see [1]), bringing theoretical conditions closer to experimental ones.

For instance, Stransky Krastanow growth in Ge/Si requires tackling wetting effects, surface energy changes with thickness, and, most importantly, strain relaxation. To account for the latter the elastic energy density must be computed at each stage of the simulation, requiring time-costly (if repeated 10^5-10^6 times, as typical in a long time-scale simulation) Finite Element Method (FEM) solutions of the elastic problem. However, a significant speed up can be obtained by replacing the "ground-truth" elastic chemical potential μ_{el} provided by FEM with the prediction supplied by a suitable neural network (NN) trained on a dataset of film profiles [2,3]. Examples illustrating the possibility to enhance both the temporal and the spatial scale will be given. While the above model is deterministic, fluctuations are known to be important under several growth conditions. Step fluctuations are a prominent example, observed at the surface of many different materials. We shall illustrate how Generative Adversarial Networks (GANs) [4,5] can be used to learn stochastic step dynamics by starting from an initially flat atomic stripe. Extensions to 3D models [6] and applications to faceted-growths and decomposition in alloys [7] will be also described.

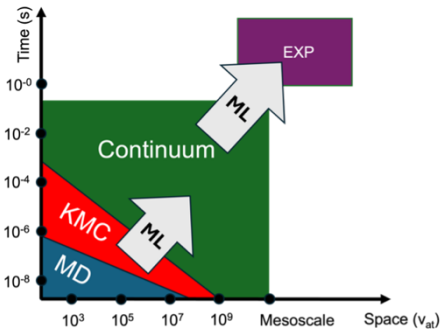

Fig. 1. Gap between experimental and theoretical conditions when attempting to simulate crystal growth by MD, KMC, or Continuum (e.g. Phase Field). ML can be exploited to reduce such gap.

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References

[1] D. Lanzoni et al., J. Phys.: Condens. Matt. **37** 403003 (2025).
[2] D. Lanzoni et al., APL Machine Learning **2**, 036108 (2024).
[3] L. Martin-Encinar et al., Comput. Mater. Sci. 249, 113657 (2025).
[4] D. Lanzoni et al., J. Chem. Phys. 159, 144109 (2023).
[5] D. Lanzoni et al. *Learning lattice Kinetic Monte Carlo stochastic surface dynamics with Deep Generative Adversarial Networks*, Acta Mat. (2026, *in press*).
[6] D. Lanzoni et al., Mach. Learn: Sci. & Technol. **5**, 045017 (2024).
[7] A. Fantasia et al., Adv. Th. & Sim. 9, e02144 (2026).