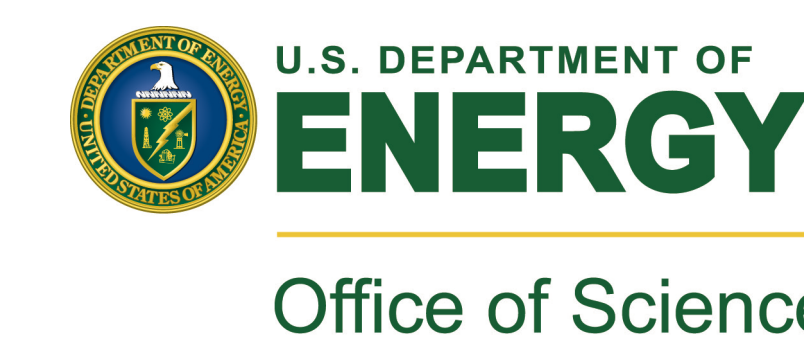




Designing thin film microstructures using genetic algorithms

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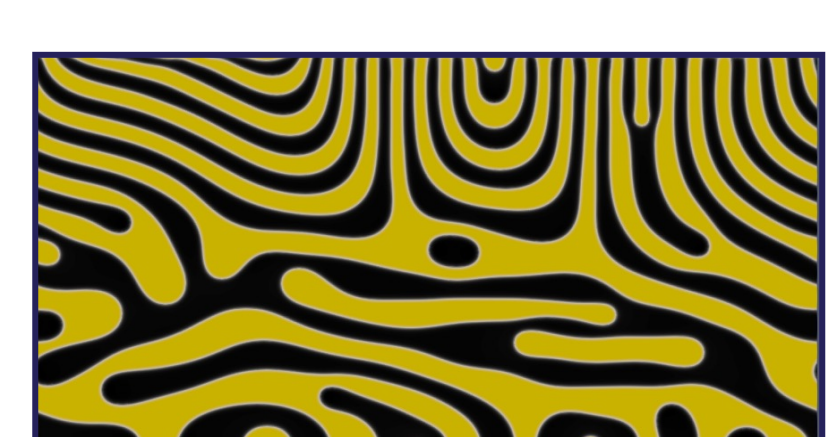


Introduction

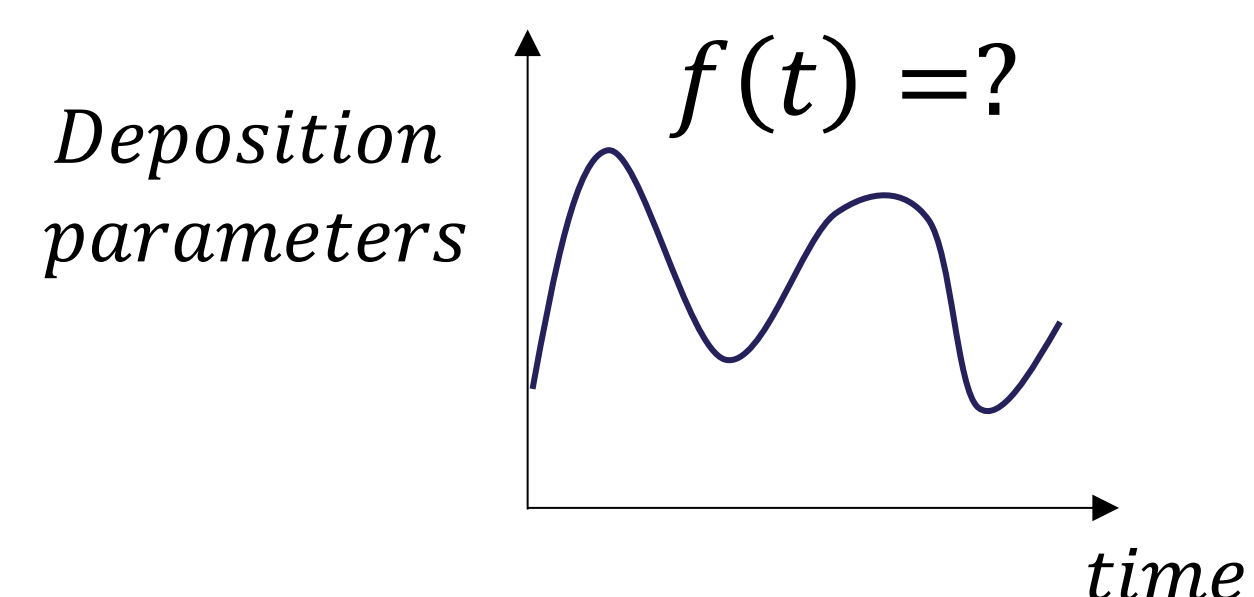
- Designing next generation thin films tailored for specific applications requires a detailed understanding of structure-processing relationships
- Traditional structure-processing mappings are low dimensional and limited in the exploration of the design space
- Phase field modeling and machine learning provide tools to predict processing conditions that achieve desired microstructures

Objective

- Couple phase field modeling and genetic algorithms to explore time-dependent processing protocols that achieve targeted microstructures

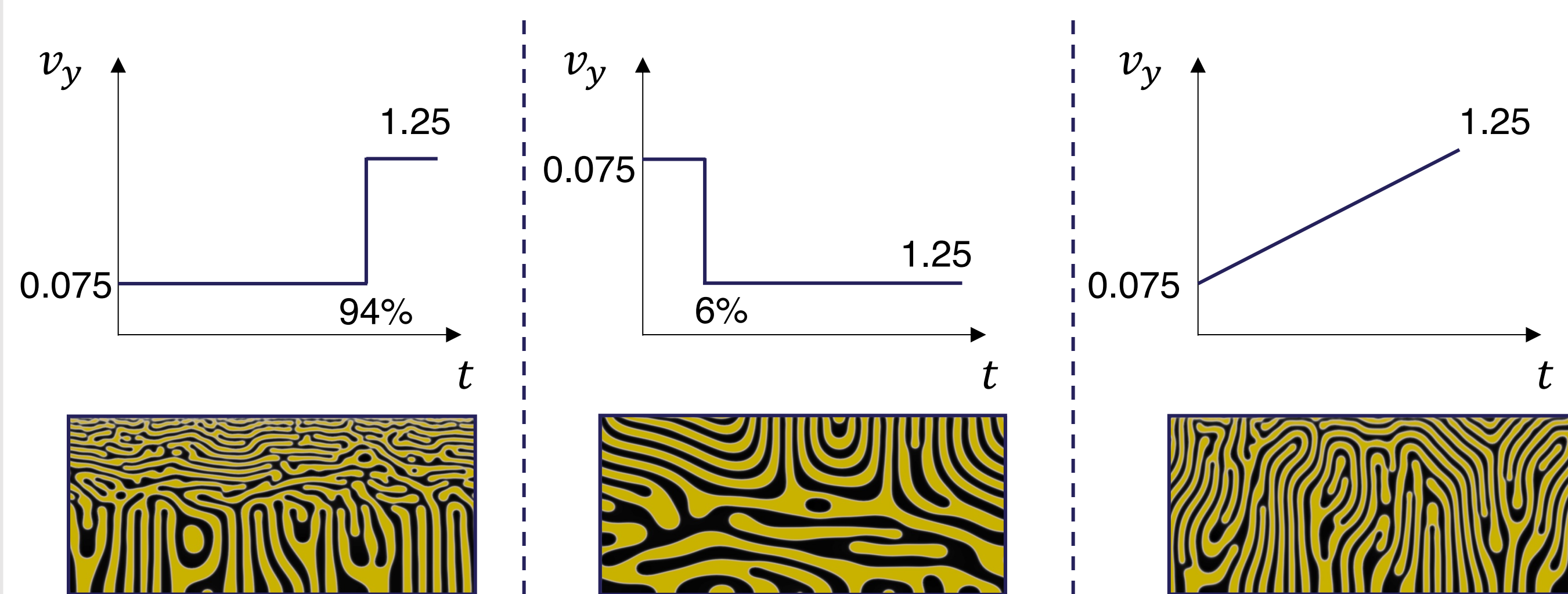


Desired microstructure



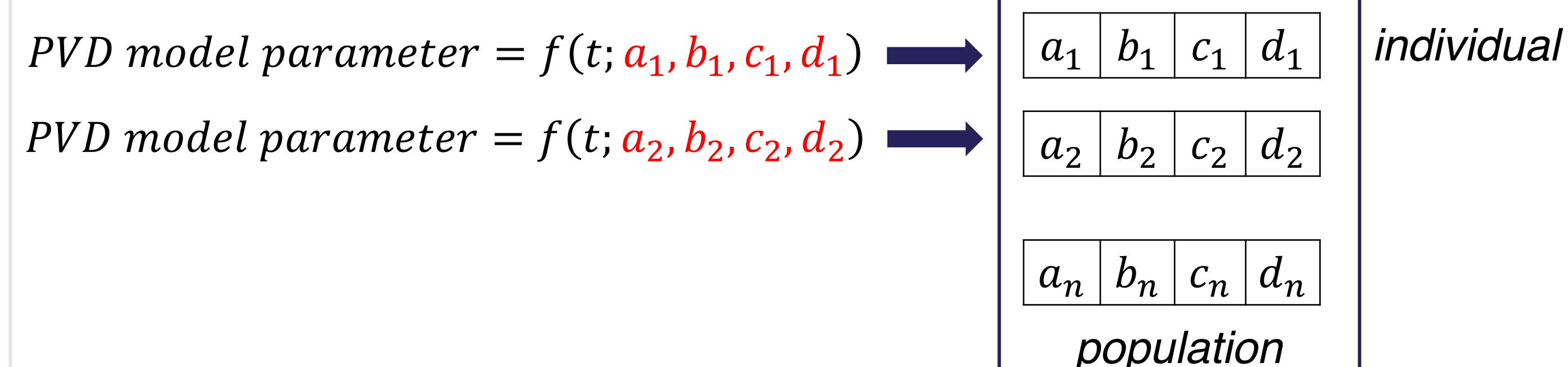
Physical vapor deposition model

Phase field code: MEMPHIS PVD model parameter $= f(t; a, b, \dots)$



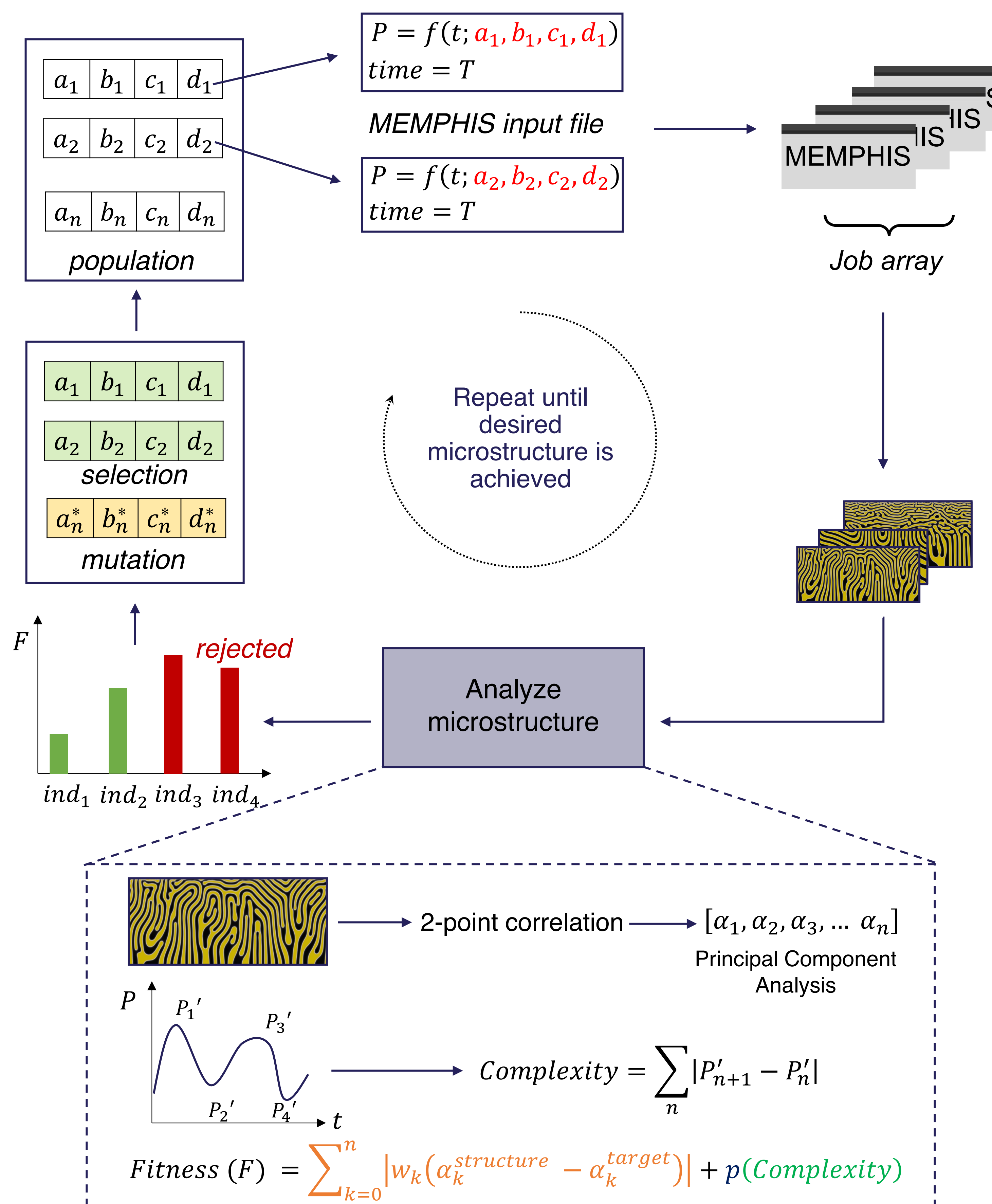
- Simple time varying protocols such as step functions and linear ramps result in hierarchical microstructures with concentration modulations
- Parameters can be specified as a Fourier series expansion to explore any time dependent processing protocol

Coupling genetic algorithms to alloy deposition

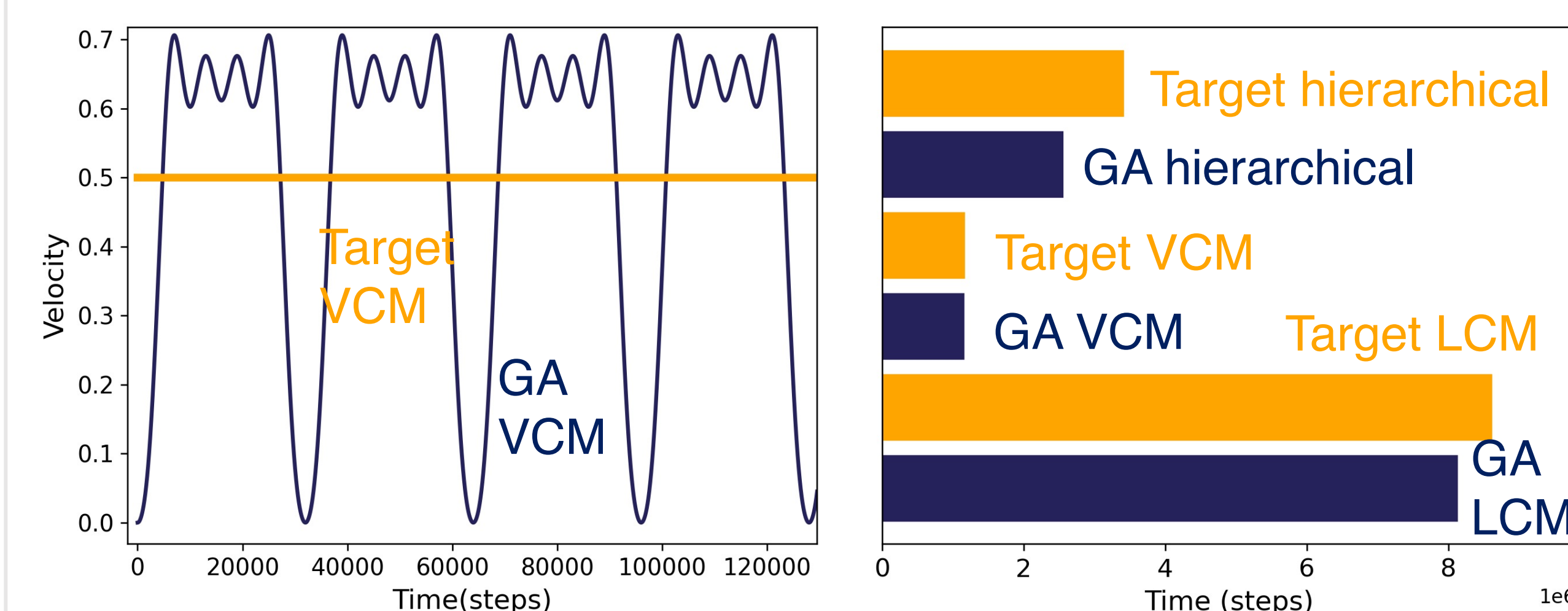


Functional form parameters encoded as individual for the genetic algorithm

Genetic algorithm guided PVD simulations

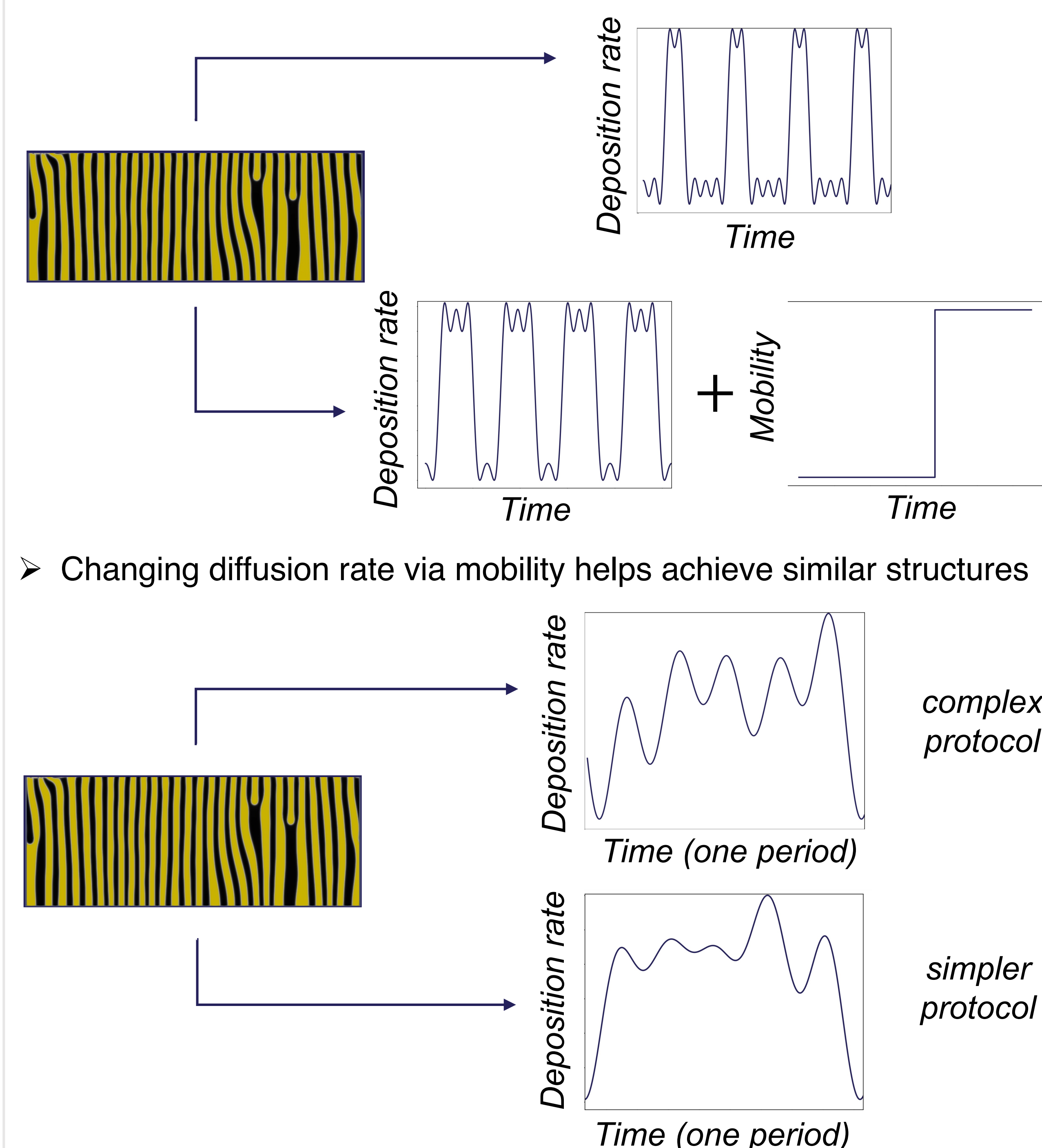


Analyzing genetic algorithm protocols



- Pulse deposition balances deposition with diffusion to achieve the same structure as constant deposition rate
- Genetic algorithm protocols achieve target structure faster

Discovering other processing protocols

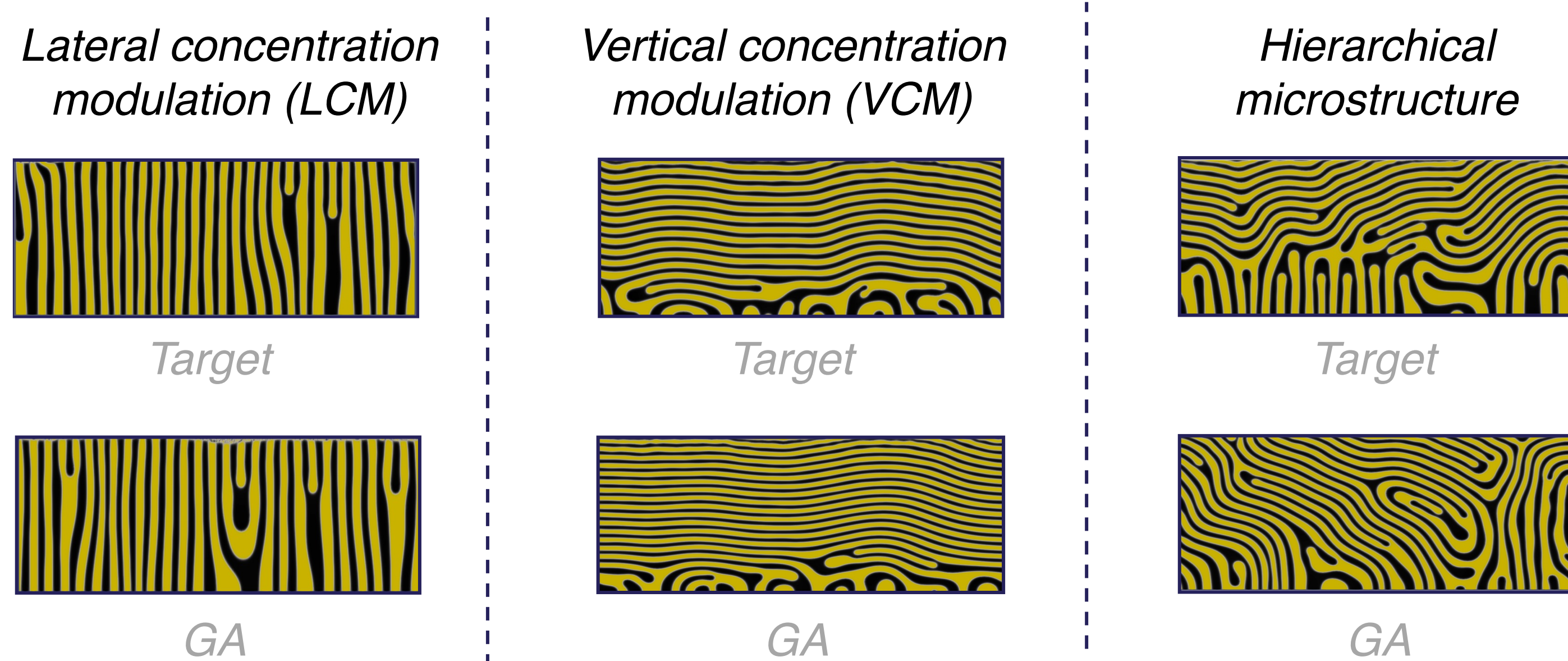


- Increasing weight on complexity term helps realize simpler protocols to achieve the same target microstructure

References

- J.A. Stewart, R. Dingreville, Acta Materialia (2020)
- E. Herman, J.A. Stewart, R. Dingreville, Applied Mathematical Modelling (2020)
- D.M. de Oca Zapiain, J.A. Stewart, R. Dingreville, npj Computational Materials (2021)

Achieving target microstructures



Genetic algorithm based protocols accurately achieve various microstructures