Multiscale simulation and AI-driven approach for advanced materials and semiconductor processing

Sung Beom Cho

Dept. Materials Science & Engineering
Ajou University

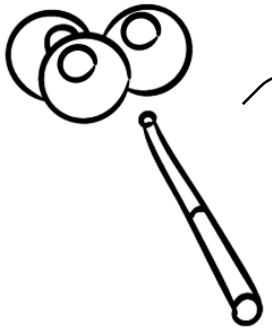
아주대학교
AJOU UNIVERSITY

What is modeling?

Complex
Real-world Problem

Understanding and
Simplifying

Mimic and predict!



You're playing
billiard

F=ma

Pick F=ma;
Neglect friction,
air resistance, …

Put the parameters;
See the trajectories

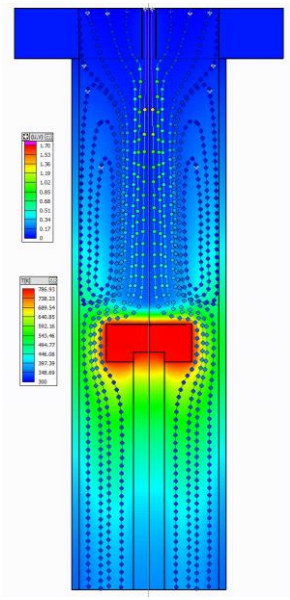
How about semiconductor process modeling?

In billiards, the trajectory from F=ma is enough. However, **materials are more complex!**

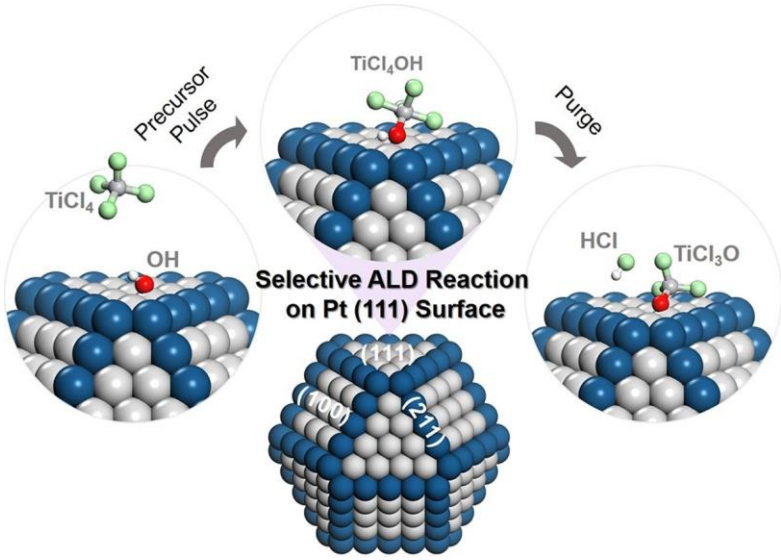
(atomic)structure process (micro)structure property applications

It cannot be described with single equation. It's Multiscale and Multiphysics problem!

Equipment

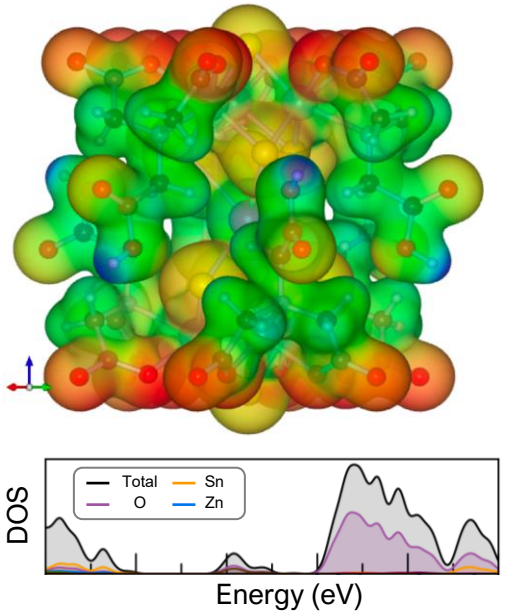


Reaction & Atomic structure

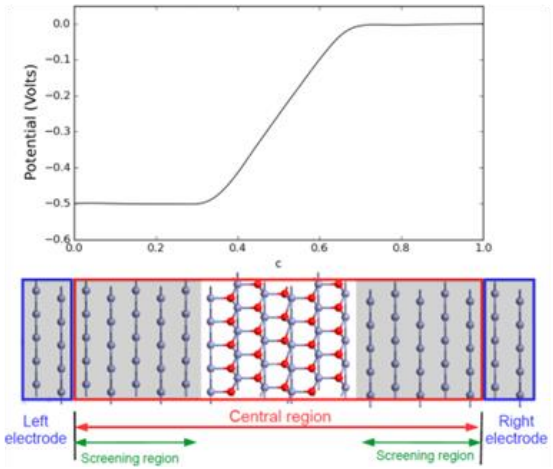


➢ 10.1016/j.apsusc.2022.154695

Electronic Structure

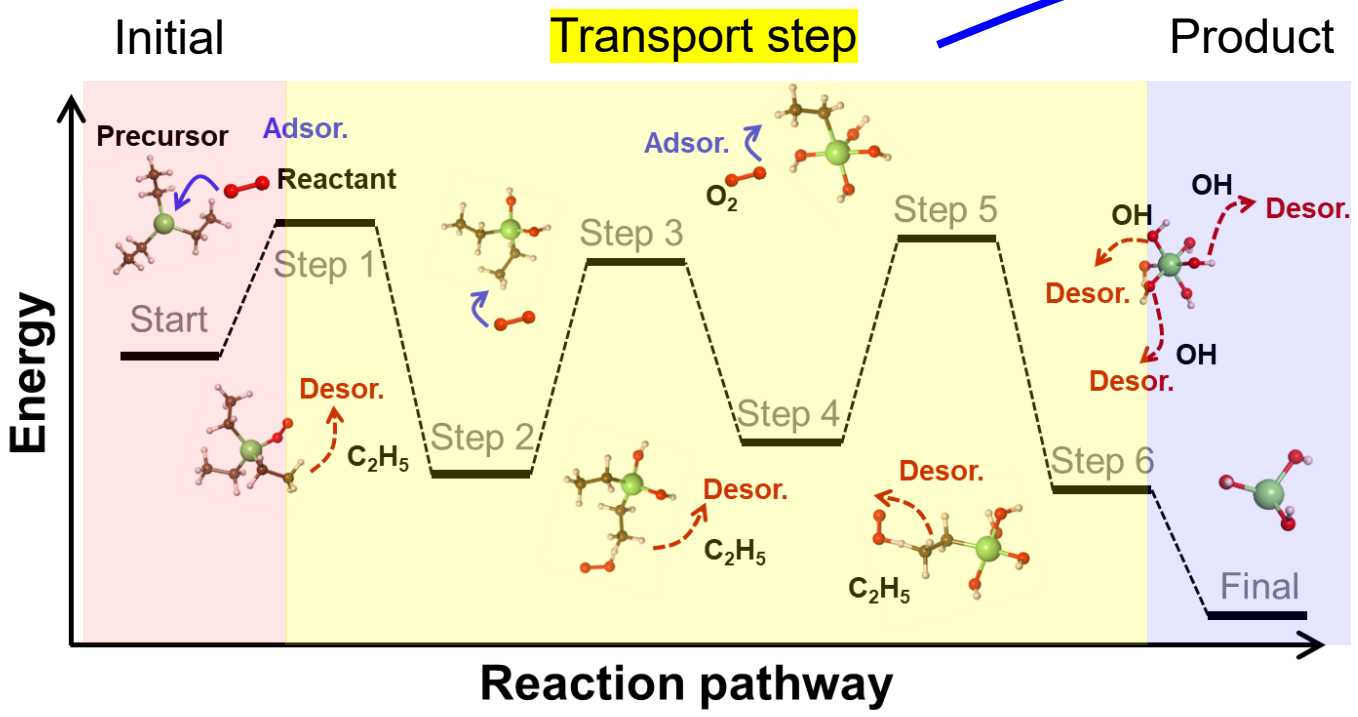


Device Property

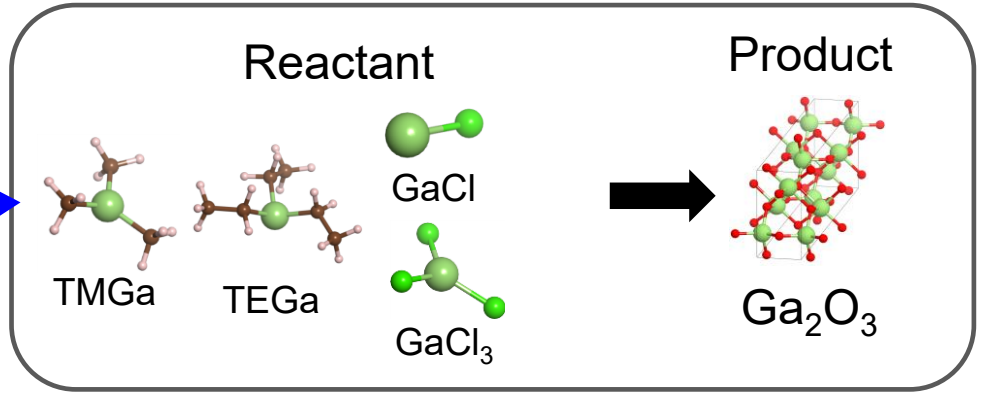


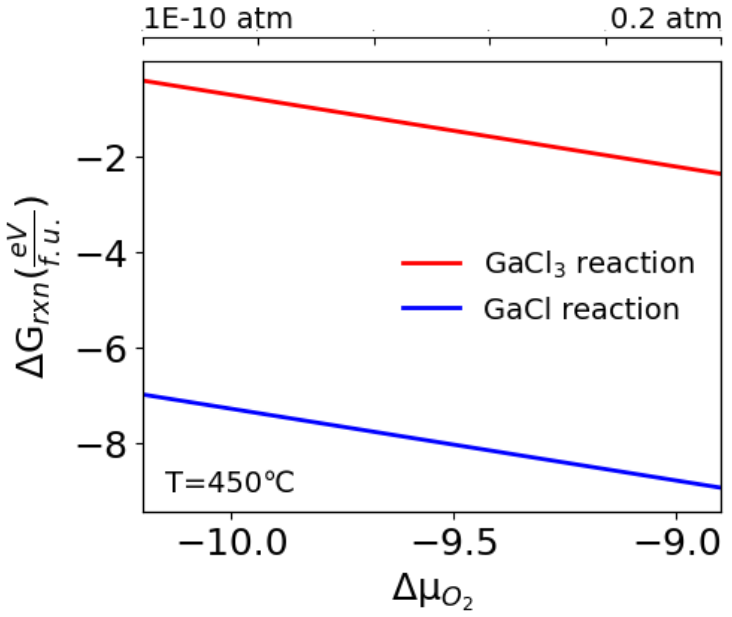
Precursor simulations (DFT)

Decomposition process of precursors



Simplify!





$$H_1\Psi_1 = E_1\Psi_1$$
$$H_2\Psi_2 = E_2\Psi_2 \longrightarrow \Delta H_{step1}$$

$$H_2\Psi_2 = E_2\Psi_2$$
$$H_3\Psi_3 = E_3\Psi_3 \longrightarrow \Delta H_{step2}$$

From the electronic structure,
We can extract reaction energetics w.r.t. T, p
Other information (electron polarity, etc.) is simplified

Nucleation theory simulation (DFT)

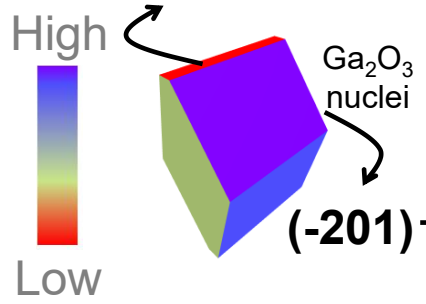
P_{O2} = 0.21 atm, Temperature ≈ 950 ℃

✓ Surface-dependent reaction energetics

$$G_{nuclei} = -n\Delta\mu + \gamma_e A_e$$

(001) ⟶ High energy

(-201) ⟶ Low energy

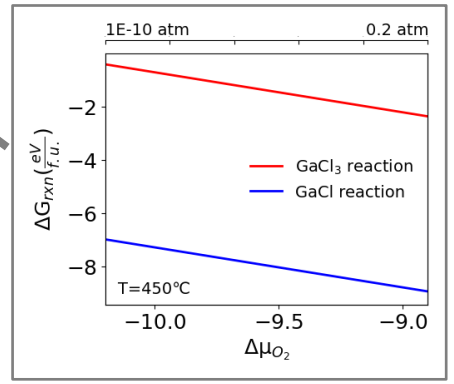


✓ Classical nucleation theory

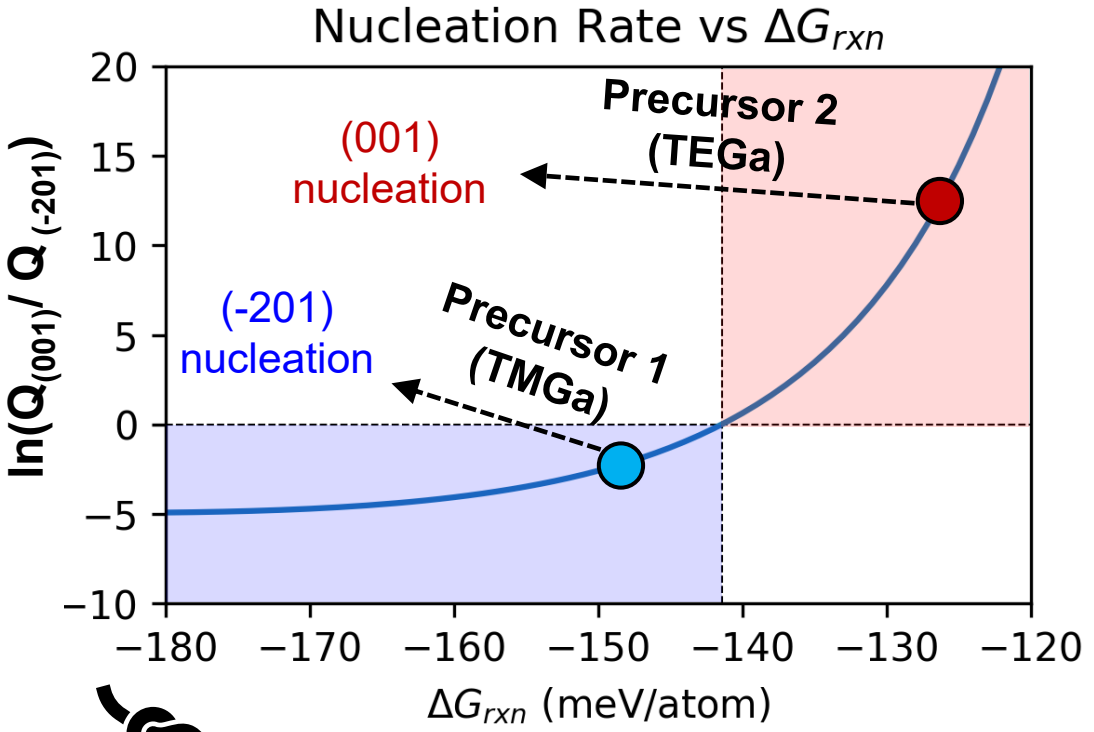
$$\mathbf{Q \approx \exp\left(\frac{16\pi\gamma^3}{3k_BT(\Delta G_{rxn})^2}\right)}$$

Knowledge

Reaction energy
(from precursor simulation)



nucleation, orientation, polymorph information can be extracted

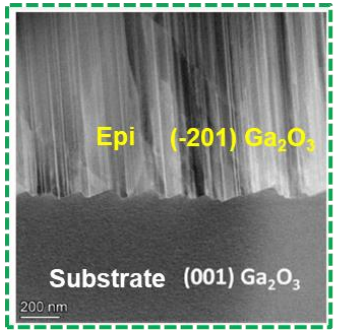


Exp.

Using TMGa

⇩

(-201) growth!

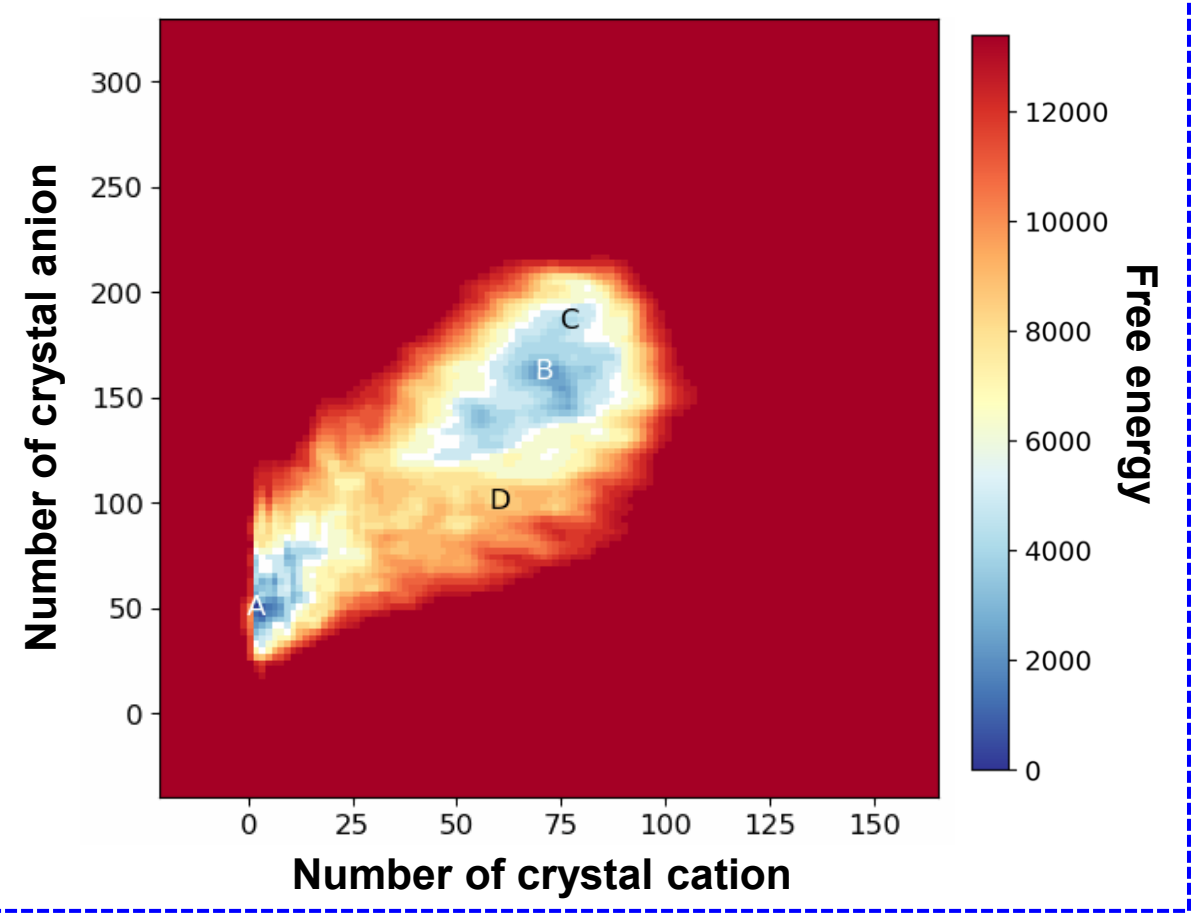


Cryst. Growth Des. 24, 3737-3745 (2024)

Nucleation kinetics analysis (MD)

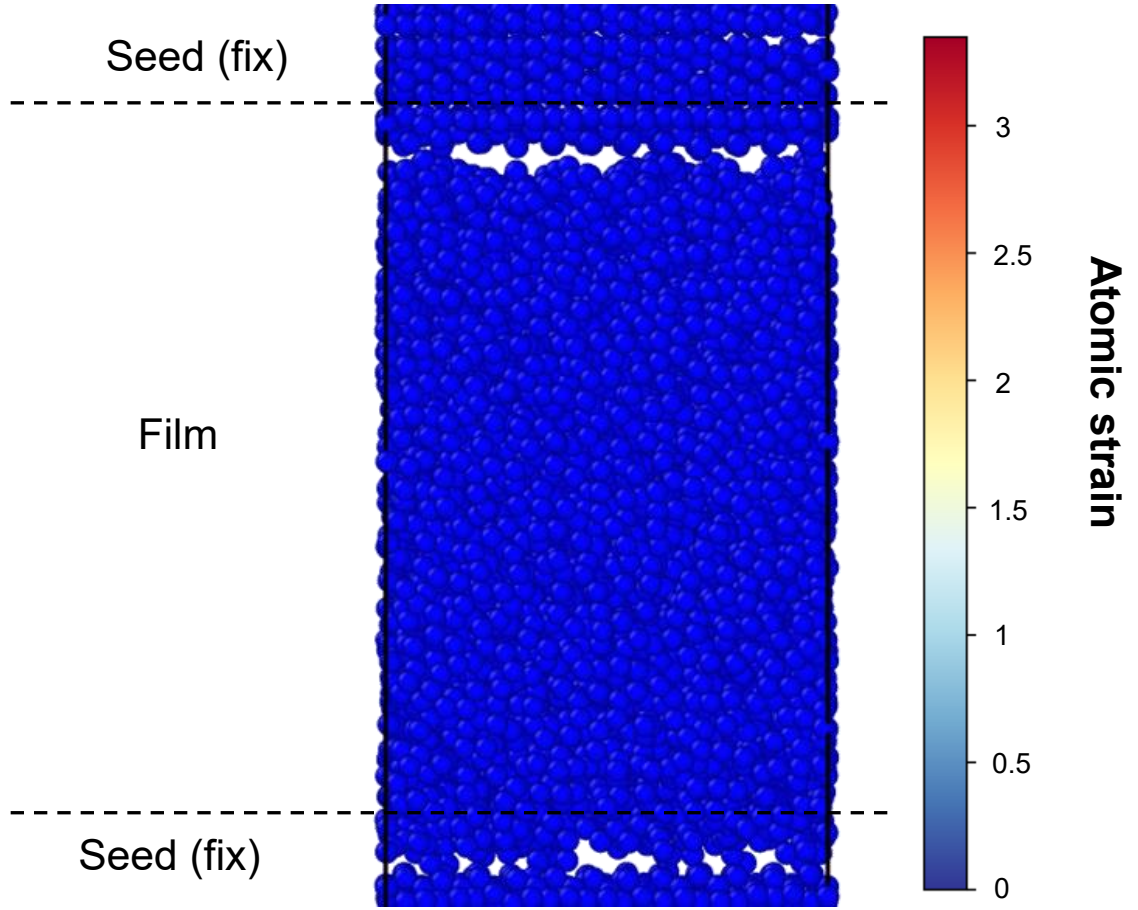
1. Nucleation free energy

Exploring nucleation path (0 ns → 10 ns)

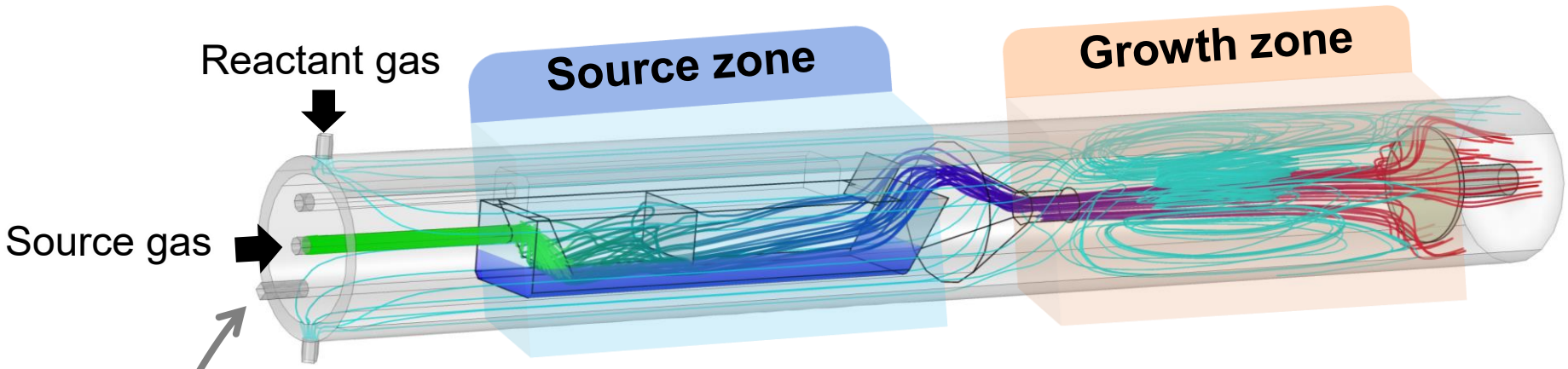


2. Interfacial strain analysis

Growth simulation (0 ns → 10 ns)



HVPE chamber modeling based on Multiphysics FEM

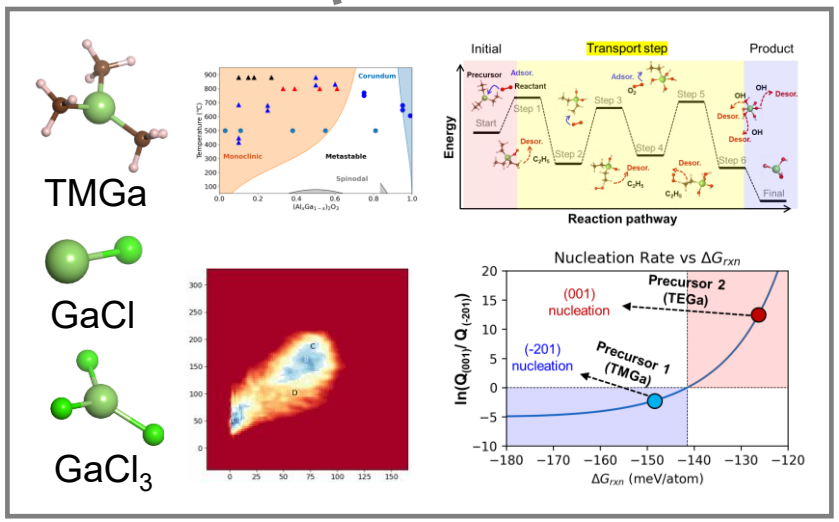


Governin Eq.

Fluid dynamics
Heat transport
Gas diffusion

Parameterized Knowledge

Variable call-up



✖ Non-selectable

- ✓ Turbulence and vortex
- ✓ Molecule diffusion
- ✓ Gas pressure
- ✓ …

Fluid-related

Selectable

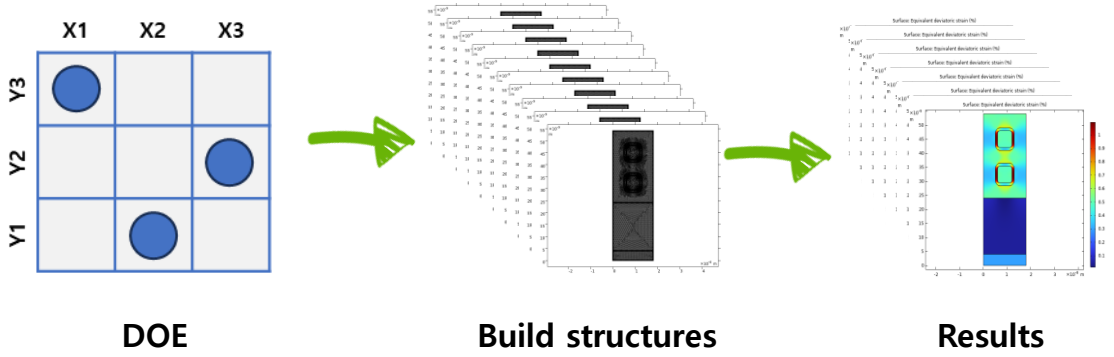
- ✓ Gas flow (N_2, sccm)
- ✓ Suspector position (cm)
- ✓ Temperature (℃)

- ✓ Temperature gradient
- ✓ Gas temperature
- ✓ Nucleation Reactions
- ✓ …

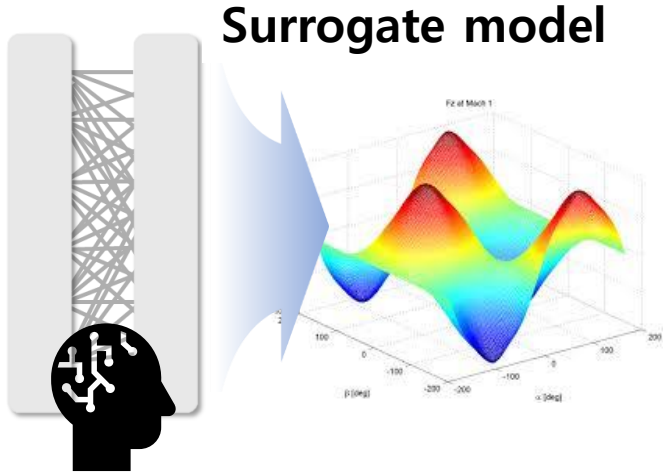
Thermal-related

Optimizing process

Parametric study (data collection)



AI modeling



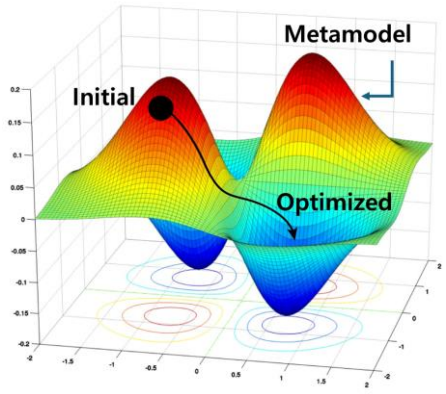
Optimization

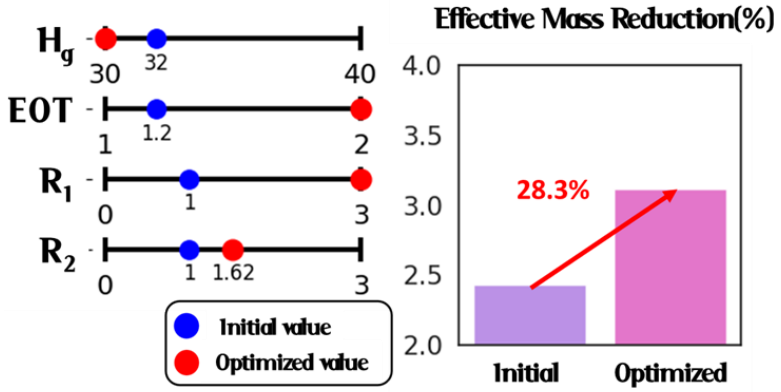
GEOMETRY PARAMETERS

- R_1 : 1-3
- R_2 : 1-3
- EOT : 1-2
- H_g : 30-40

TARGET PROPERTY

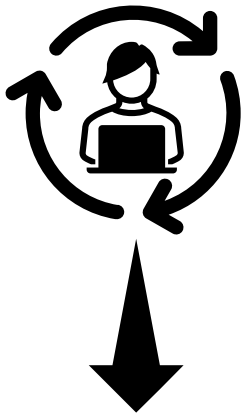
- Effective mass : Minimizing



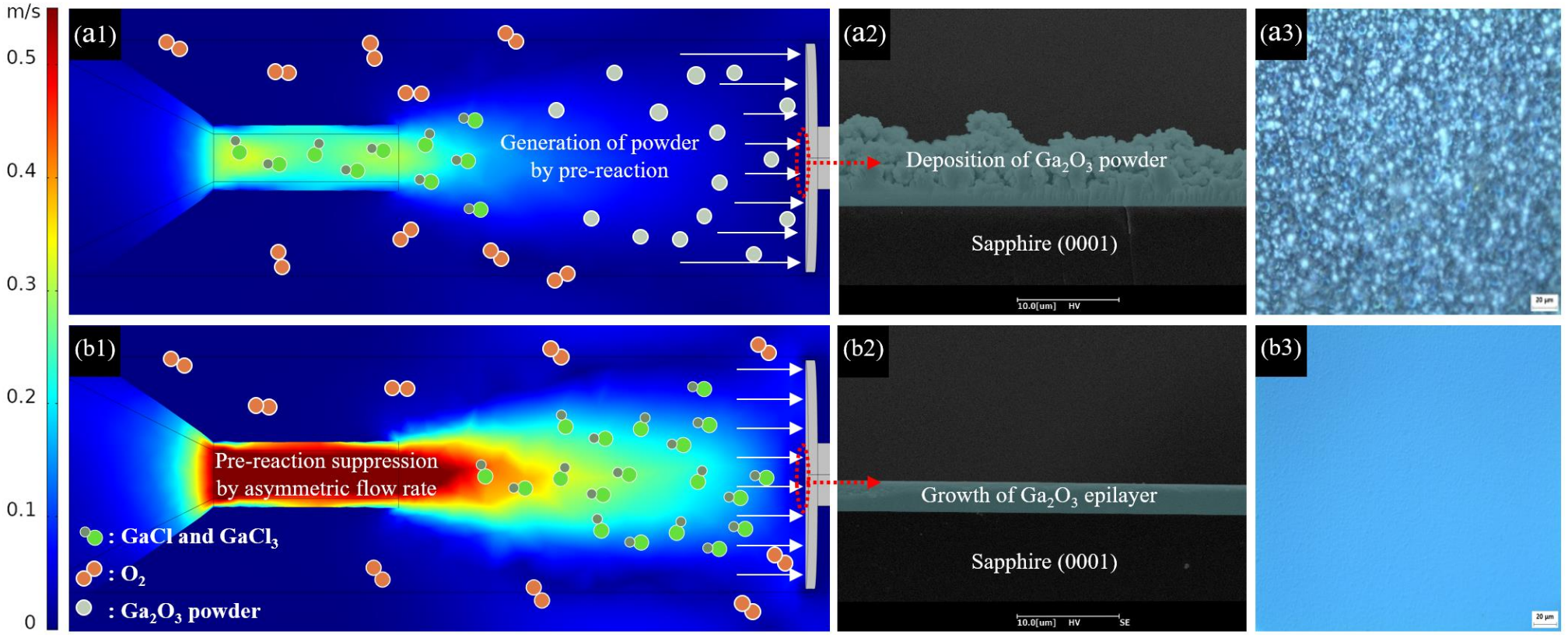


Experimental validation on deposition quality

Computation



Optimization!



Gas velocity in growth zone **SEM** **OM image**

Concluding Remarks

- The key idea of modeling is capturing essential physics in complex by simplifying the phenomena
- For real problem, we need to solve multiple governing equations in multiscale & multiphysics dimension
- We have constructed AI-assisted simulator to get optimized recipe