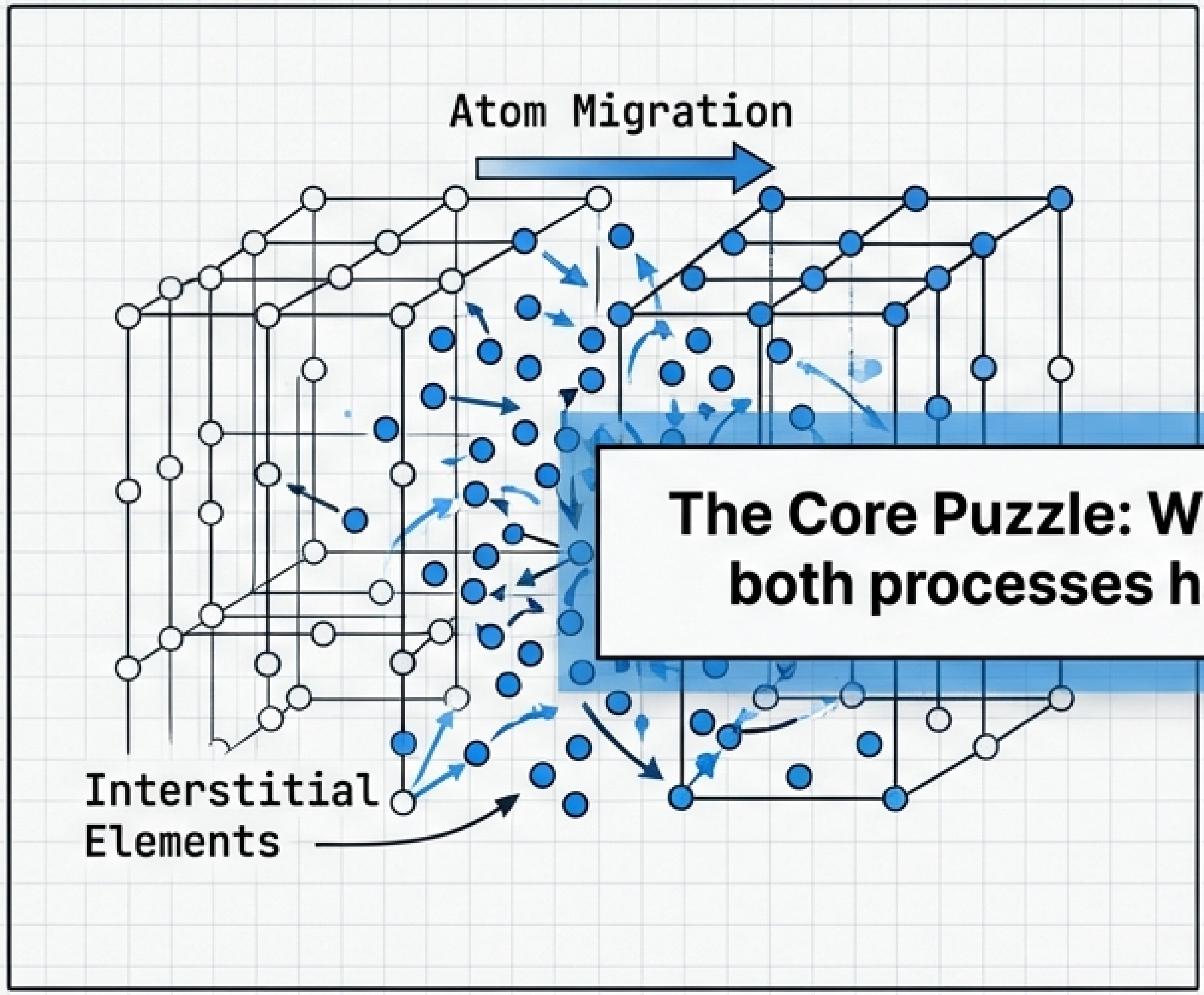
The Thermodynamic Blueprint

Coupling Diffusional and Displacive Transformations in Steel

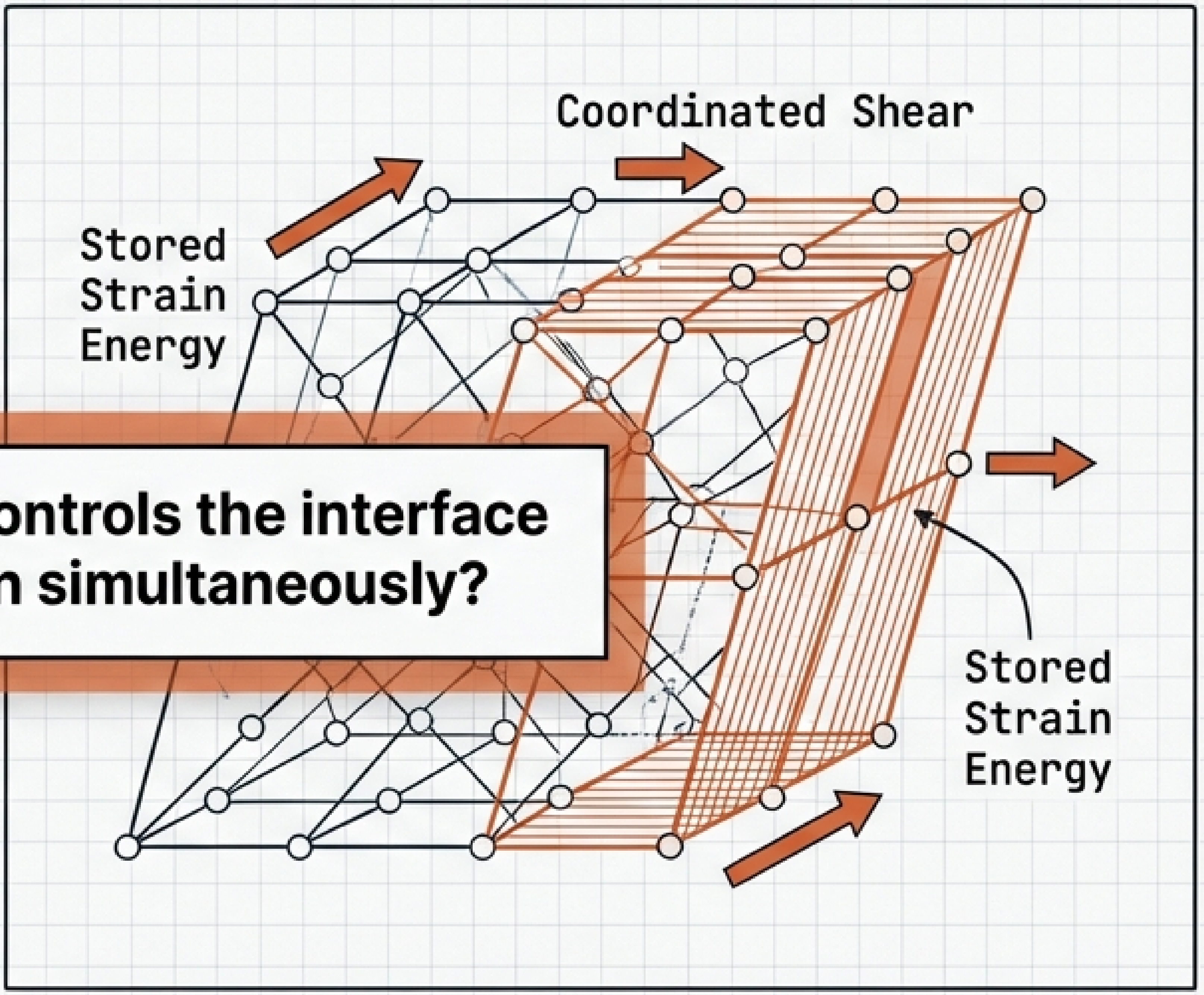
A visual synthesis of the Olson, Bhadeshia, and Cohen model.

Diffusional Transformations



- Atom-by-atom transfer across the interface.
- Partial redistribution of interstitial elements (Carbon).

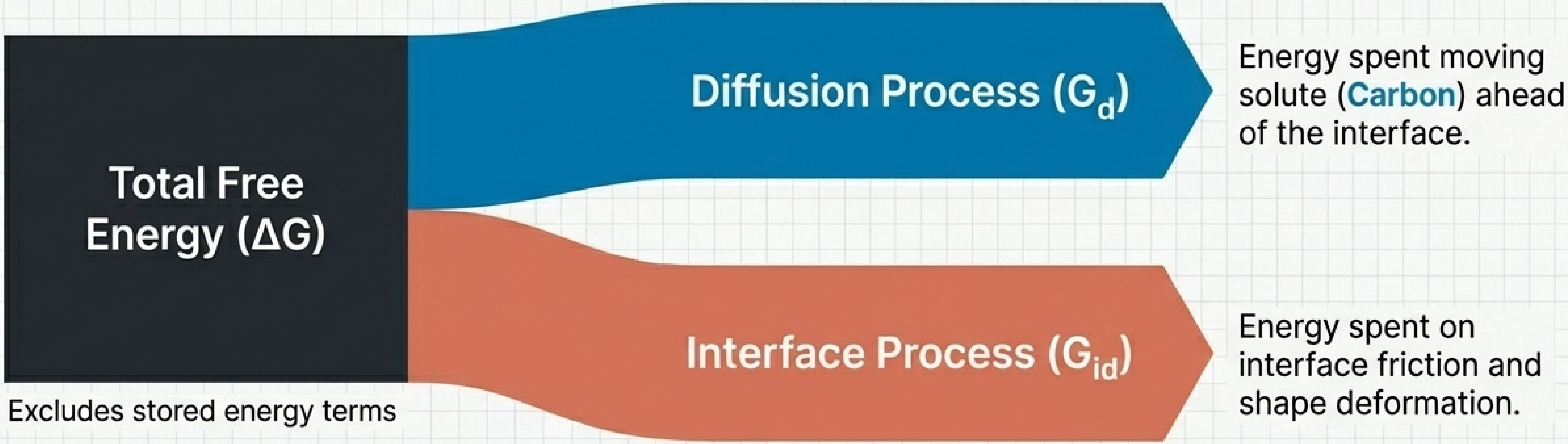
Displacive Transformations



- **Coordinated lattice shear** (e.g., $\gamma \rightarrow \alpha$ martensite).
- No substitutional diffusion; dependent on stored strain energy.

The Core Puzzle: What controls the interface both processes happen simultaneously?

The Thermodynamic Energy Budget



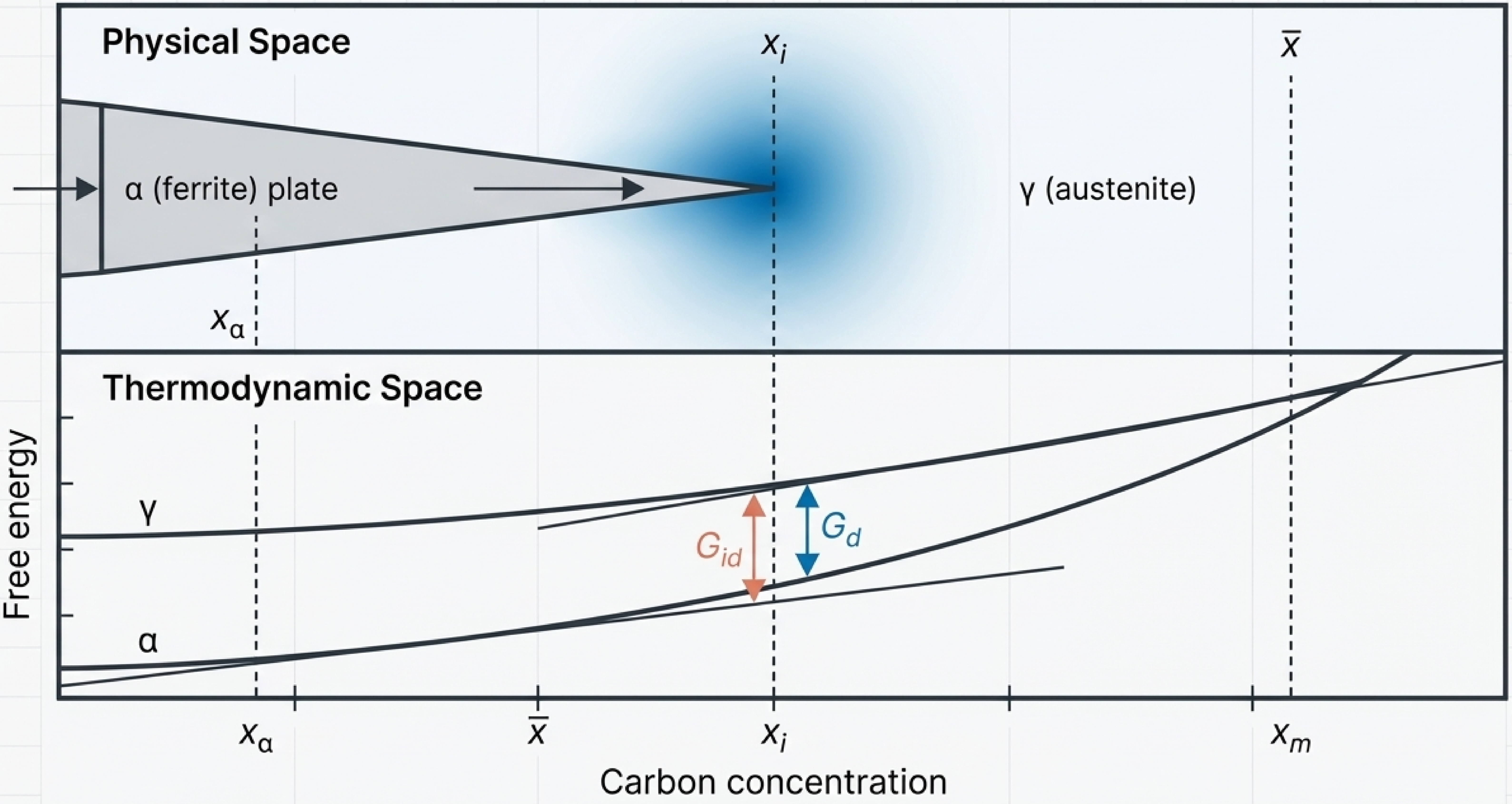
$$\Delta G = G_d + G_{id}$$

Diffusion-Controlled: $\Delta G \approx G_d$

Interface-Controlled: $\Delta G \approx G_{id}$

Mixed Control: Neither dominates

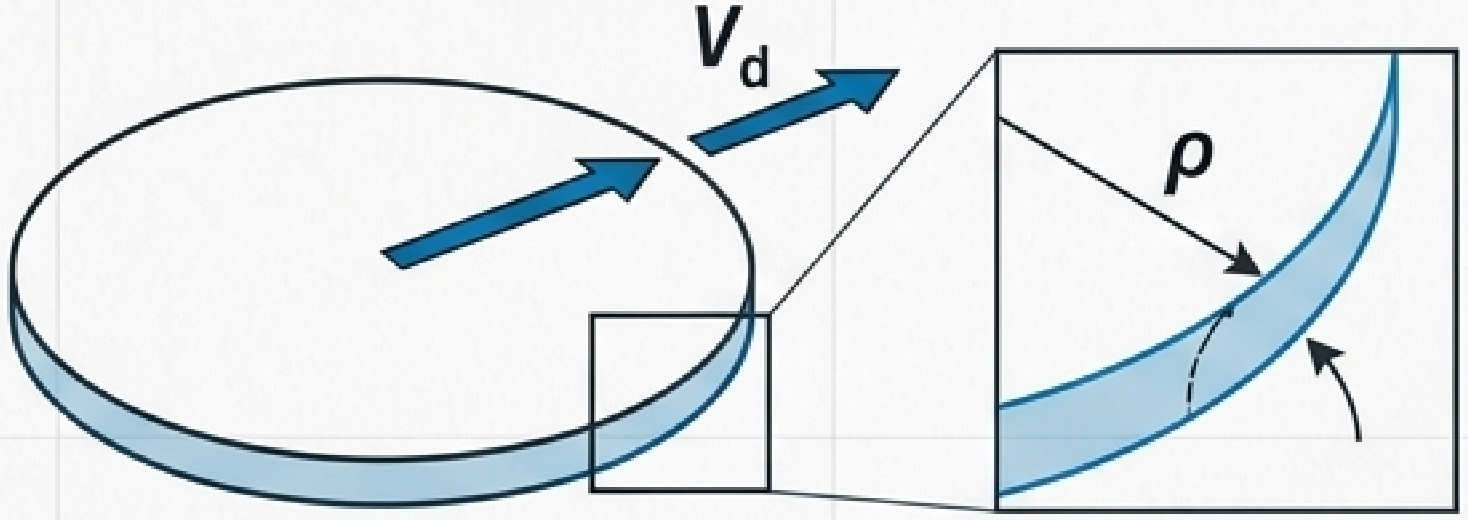
Mapping Physical Space to Phase Space



The Diffusional Engine: Carbon Evacuation

$$V_d = \psi(G_d)$$

Physical Geometry



Model assumes a disc-shaped particle advancing at velocity V_d.

The Mathematical Limits

Ivantsov Equation

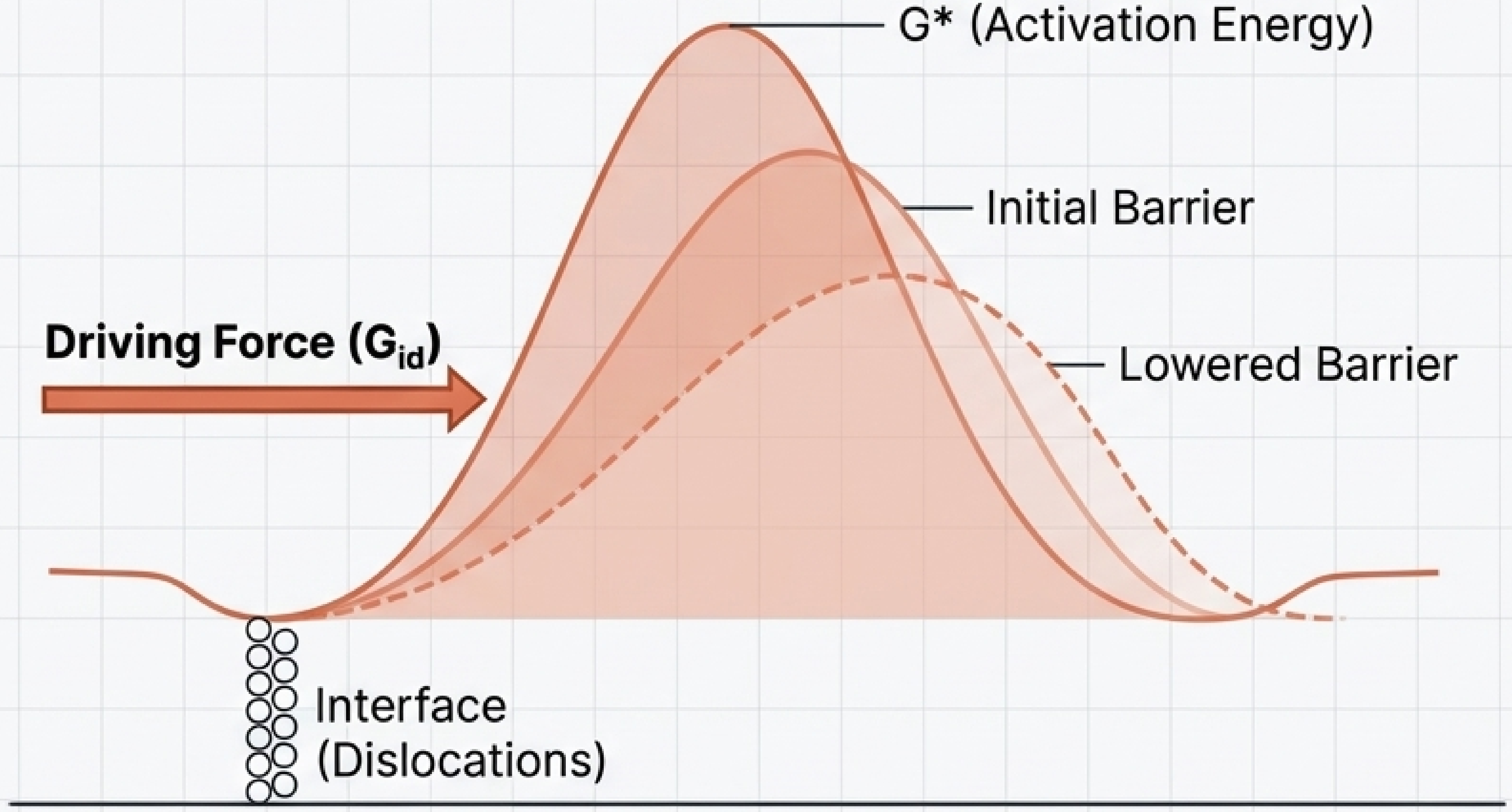
$$\frac{\bar{x} - x_\alpha}{x_\alpha - x_i} = (\pi p)^{0.5} \exp\{p\} \operatorname{erfc}\{p^{0.5}\}$$

Péclet Number

$$p = \frac{V_d \rho}{2\bar{D}_{bar}}$$

Insight: To calculate V_d, we fix G_id and G_d. The diffusion coefficient D_bar depends heavily on carbon concentration, making this limit highly dynamic.

The Displacive Engine: Thermal Activation



Thermal Activation Equations

Velocity:

$$V_i = V_0 \exp[-G^*/(kT)]$$

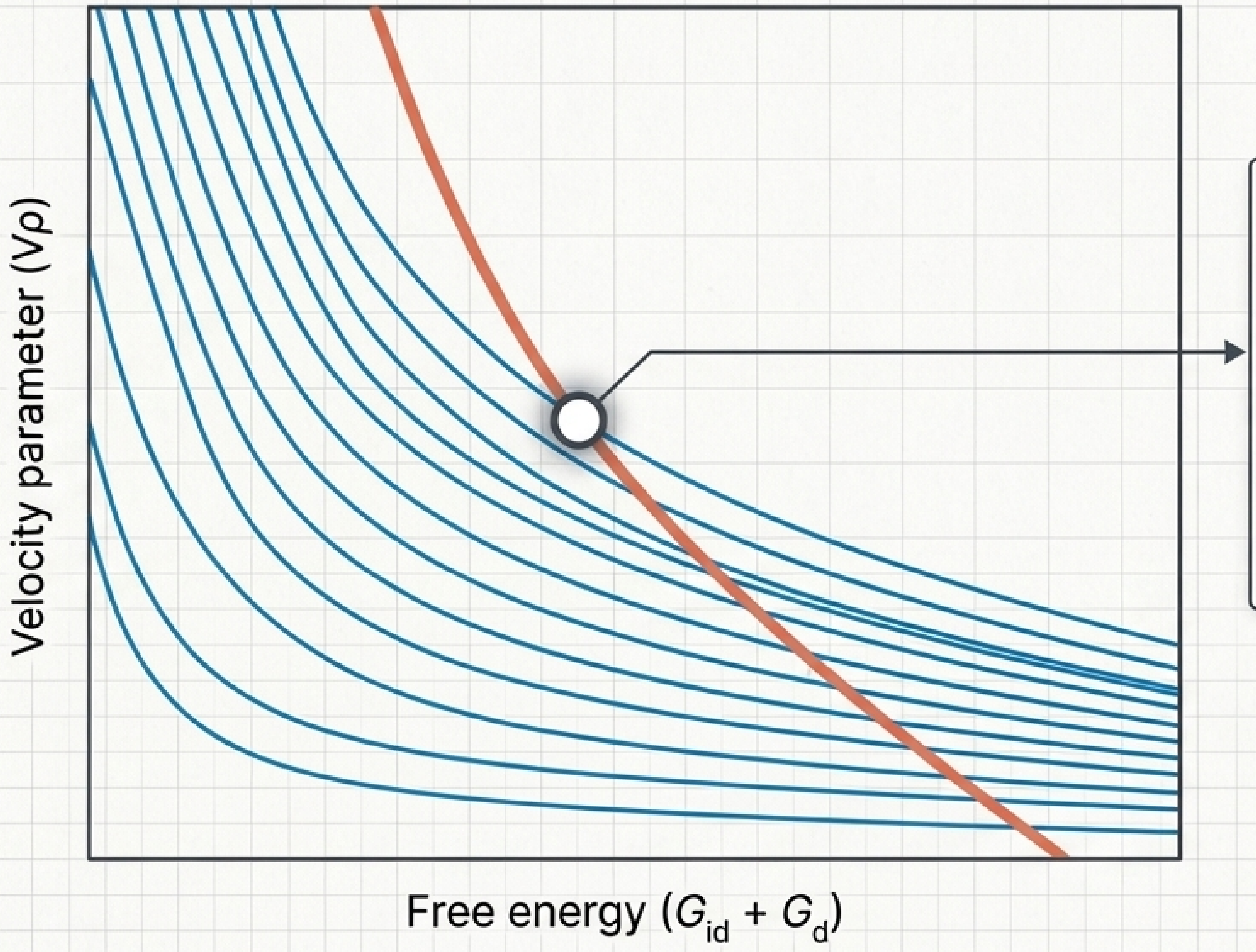
(V_0 = 30 m/s dislocation limit)

Activation Barrier:

$$G^* = G_0 \left[1 - \left(\frac{G_{id}}{\hat{G}_d}\right)^y\right]^z$$

Insight: The interface moves by overcoming obstacle interactions. Speed is strictly dictated by the available driving force G_id lowering the activation barrier.

The Synthesis: The Coupling Point



The Coupling Point:

$$V_i = V_d = V$$

Growth velocity is locked exactly where energy dissipated by carbon diffusion perfectly matches the energy required to advance the crystal interface.

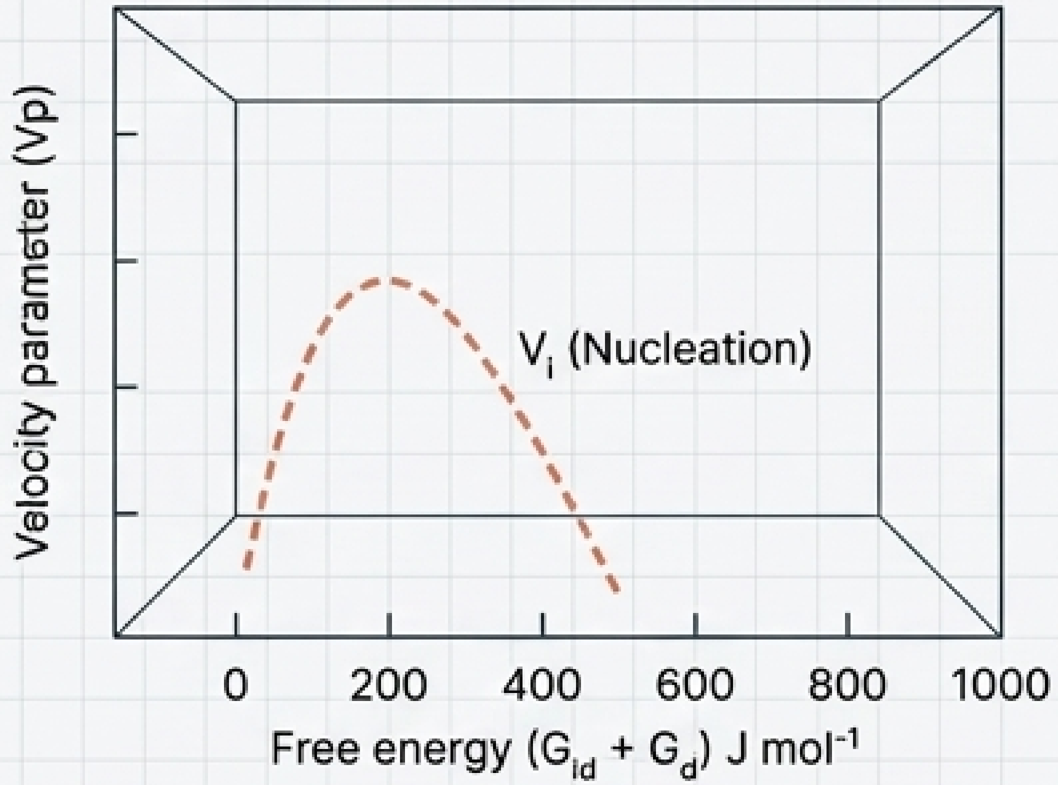
Diagnostic Matrix: The Limiting Regimes

	Diffusion-Controlled Growth	Interface-Controlled Growth	Mixed Control (Coupled)
Condition	$\Delta G \approx G_\mathrm{d}$	$\Delta G \approx G_\mathrm{id}$	$V_\mathrm{i} = V_\mathrm{d}$
Velocity Limit	$V = \psi(G_\mathrm{d})$	$V = \xi(G_\mathrm{id})$	Equilibrium Intersection
Physical State	Interface mobility is high. Growth is entirely bottlenecked by how fast carbon can clear out of the way.	Carbon diffusion is rapid. Growth is bottlenecked by the inherent friction of the $\gamma \rightarrow \alpha$ lattice transformation.	Delicate thermodynamic balance governing the formation of bainite and Widmanstätten ferrite.

Thermodynamic Constraints: Nucleation vs. Growth

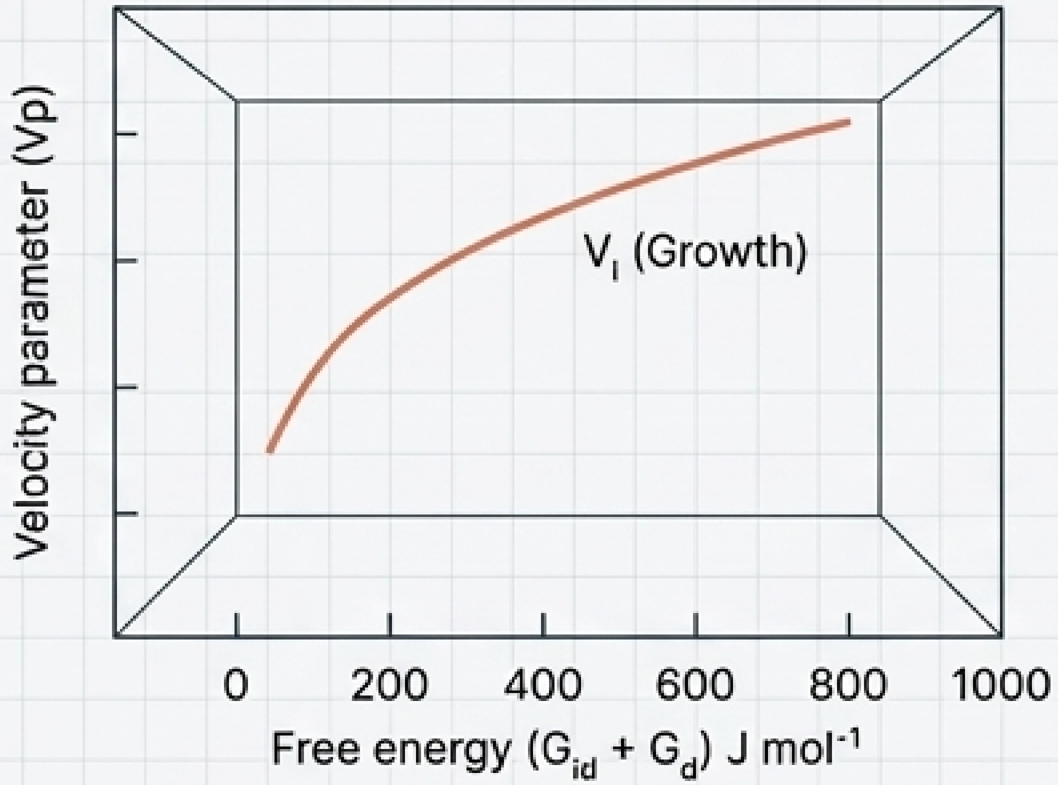
Nucleation Phase

- **Energy Barrier:** Requires immense stored energy (>700 J/mol) to initiate.
- **Kinetics:** Velocity passes through a maximum as temperature decreases (classic C-curve behavior).

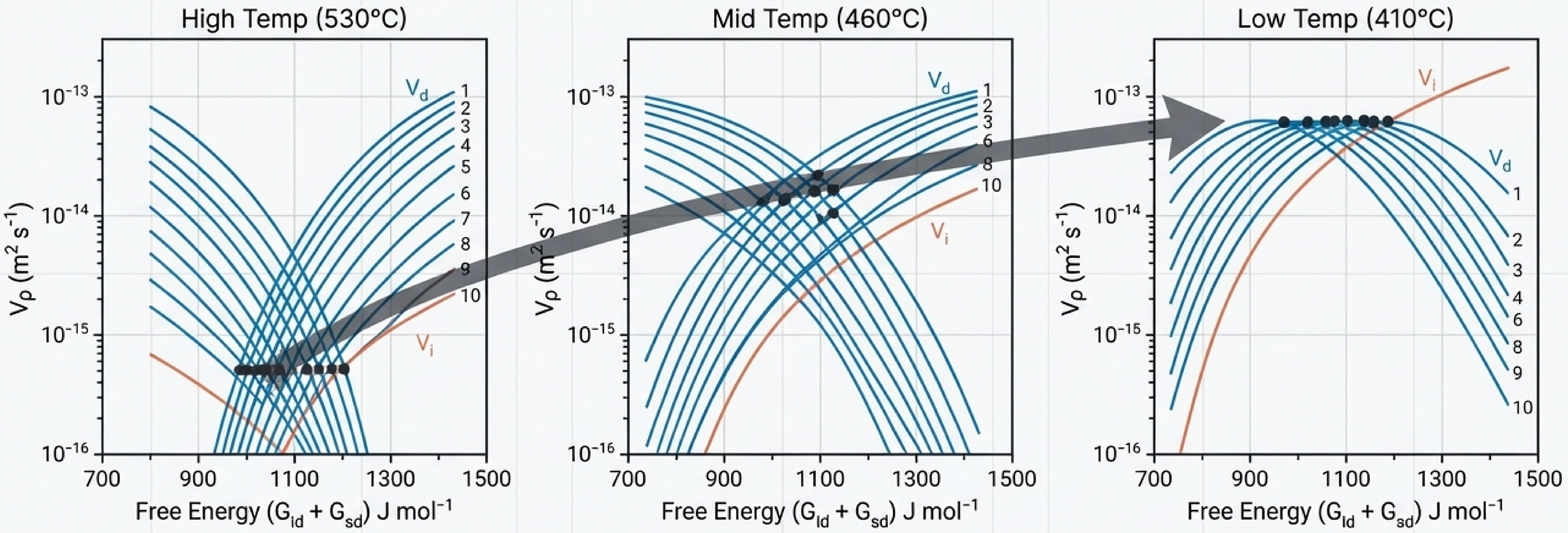


Growth Phase

- **Energy Barrier:** Stored energy drops significantly due to plastic accommodation of subunits.
- **Supersaturation:** Full supersaturation is thermodynamically permissible above the M_s temperature.

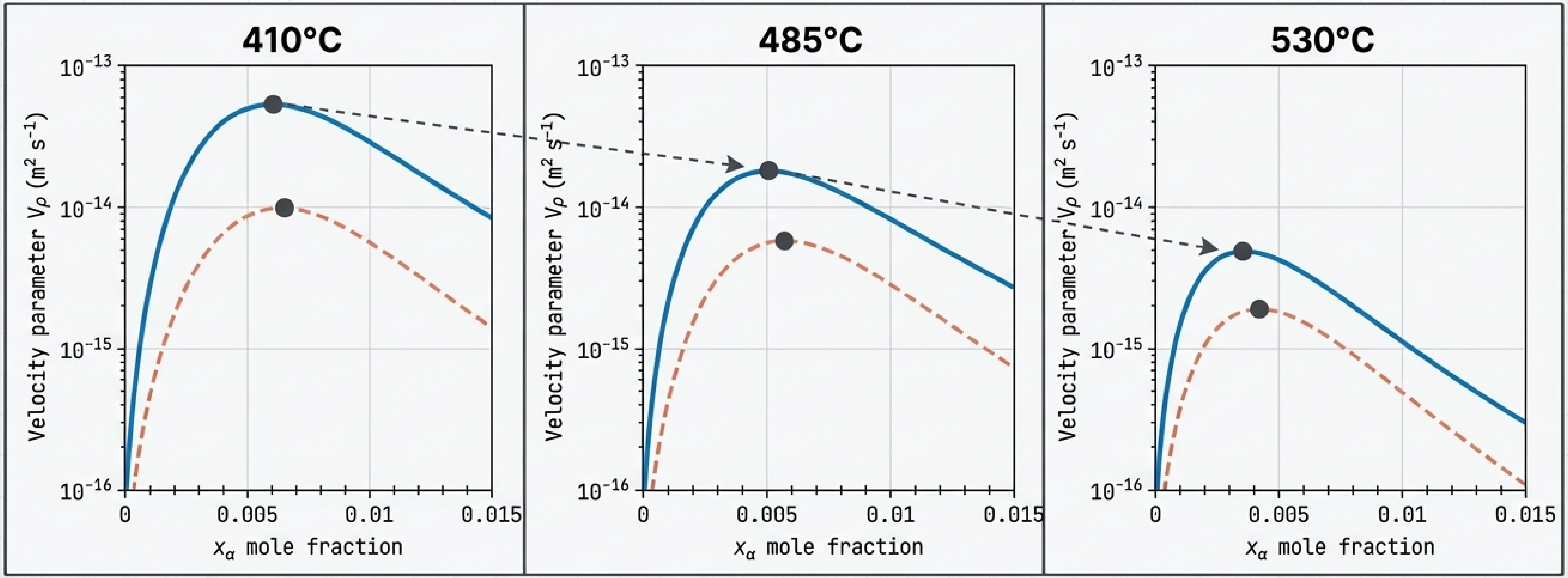


Temperature Impact on Thermodynamic Balance



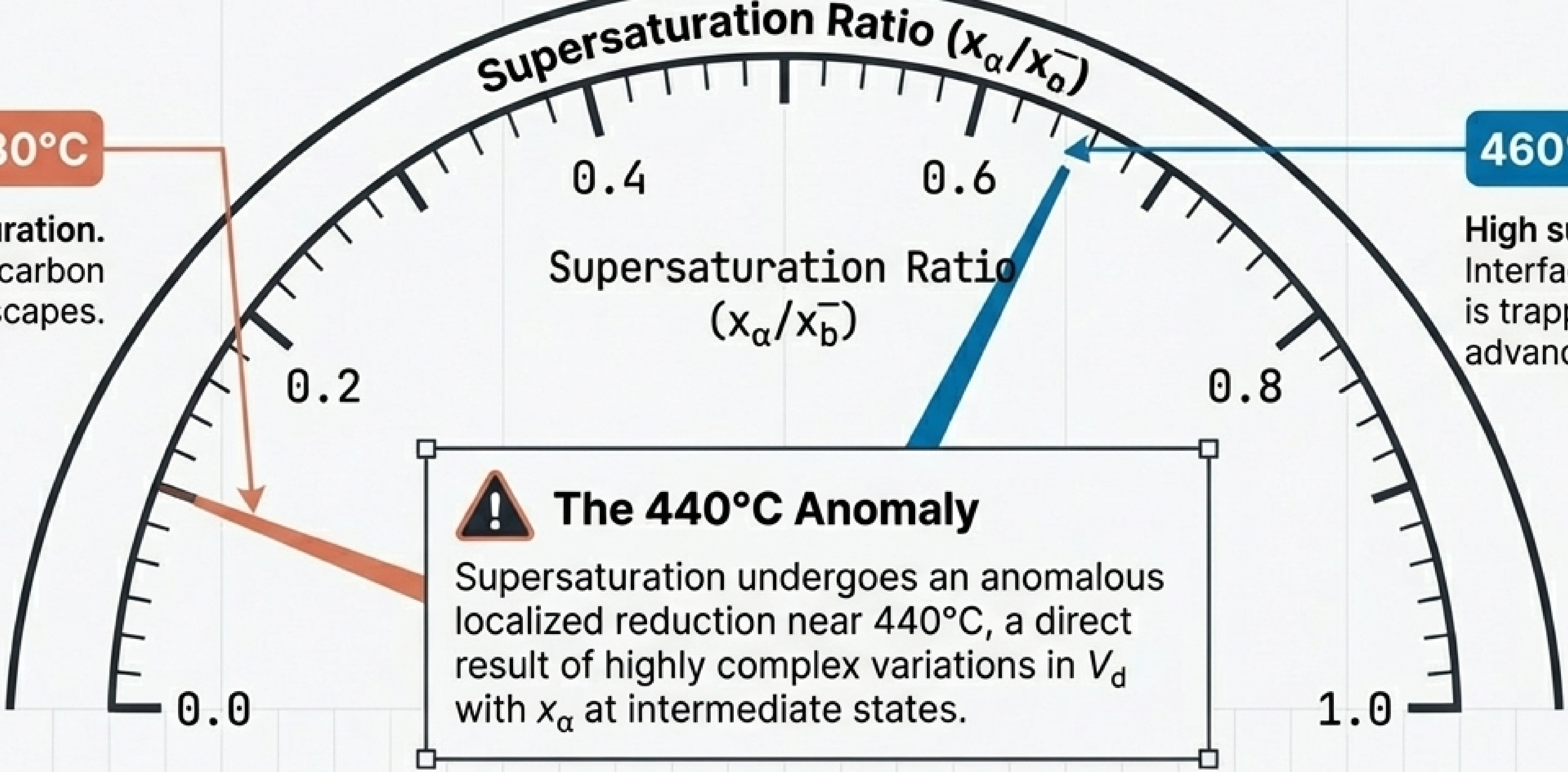
Insight: As transformation temperature decreases from 530°C to 410°C, the peak growth rate of a plate (V_{max}) increases monotonically.

C-Curve Kinetics: Identifying Maximum Velocity



Assumption: Transformations occur at the specific carbon concentration (x_α) corresponding to the absolute maximum growth rate. High temperatures reduce this velocity despite easier carbon diffusion.

Outcome: Carbon Supersaturation Predictions



Low supersaturation. Interface is slow; carbon successfully escapes.

High supersaturation. Interface is fast; carbon is trapped in the advancing lattice.

The 440°C Anomaly

Supersaturation undergoes an anomalous localized reduction near 440°C, a direct result of highly complex variations in V_d with x_α at intermediate states.

Conclusion: The coupled model successfully predicts that as transformation temperature drops, the lattice shears faster than interstitial carbon can diffuse away.

The Unified Theory of Microstructures

Martensite	Bainite	Widmanstätten Ferrite
Displacive dominance. Diffusionless nature aligns exactly with models below 410°C where the nucleation limit falls far left.	The ultimate mixed-control regime. A delicate, coupled balance between shear kinetics and solute partitioning.	High reliance on diffusion. Solute partitioning dominates the energy budget.
Left Block	Center Block	Right Block

By equating interface mobility with solute diffusion limits ($V_i = V_d$), this model provides a singular, predictive mathematical rationale for all displacive transformations in steel, permanently bridging the historical gap between diffusional and shear thermodynamics.