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Connecting Microstructure and Micromechanics

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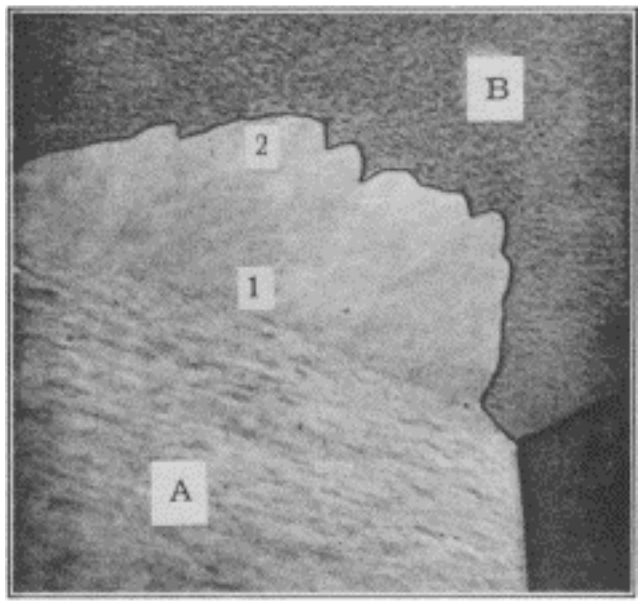
Motivation:
Stress-Induced Grain Boundary Migration

•Grain boundaries move not only to minimize interfacial energy, but also to minimize stored elastic and plastic strain energy.

Example: Stress-induced grain boundary migration (SIGBM) in aluminum

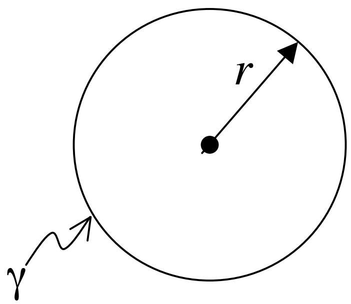


R. E. Reed-Hill, *Physical Metallurgy*, 1973.

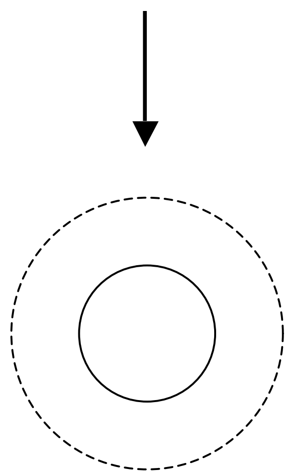
•Can microstructural models capture the interaction between grain structure and mechanical state?

Evolution mechanisms in SIGBM

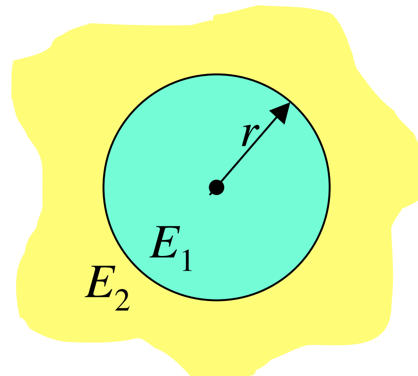
Curvature



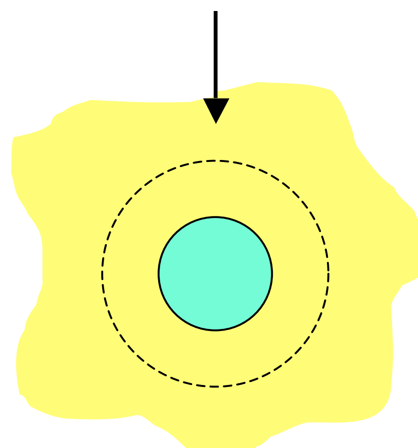
$$v_\kappa = -M_\kappa \gamma \kappa$$



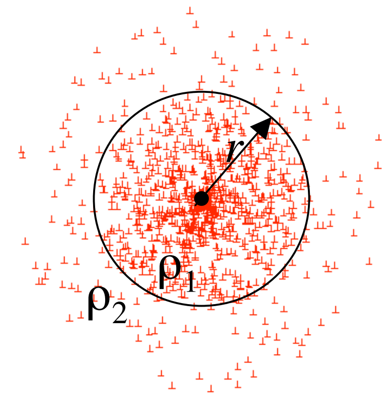
Elastic Energy



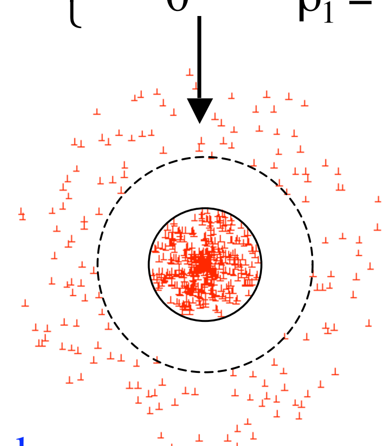
$$v_\varepsilon = M_\varepsilon \left(E_2 - E_1 \right)$$



Defects



$$v_\perp = \begin{cases} -M_\perp F_\perp \rho_1 & \rho_1 > \rho_2 \\ M_\perp F_\perp \rho_2 & \rho_1 < \rho_2 \\ 0 & \rho_1 = \rho_2 \end{cases}$$



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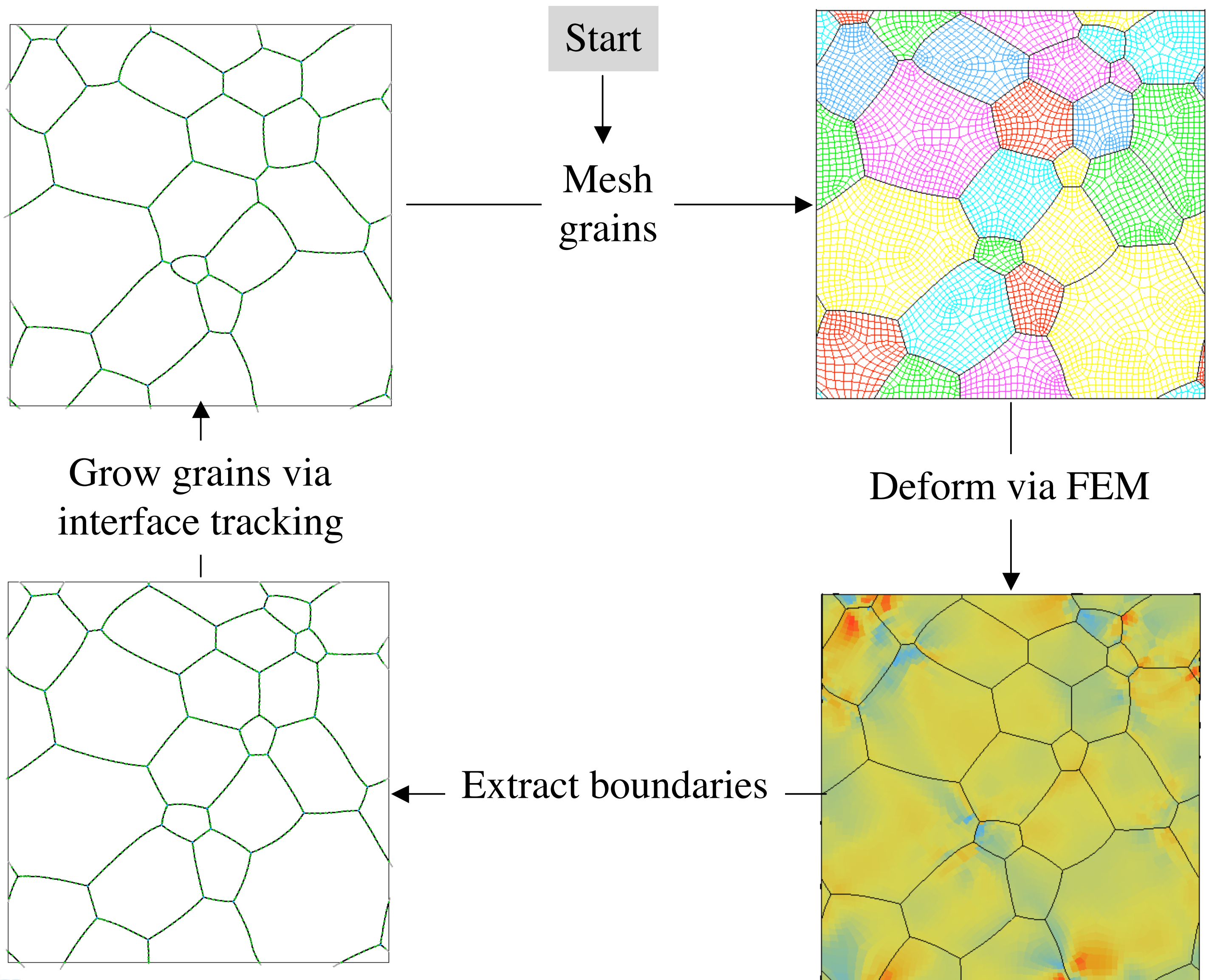
*Each mechanism also causes stresses to be re-distributed.

Schematic of fully-coupled SIGBM model



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Grain growth and stress evolution in 1% tensile hold test

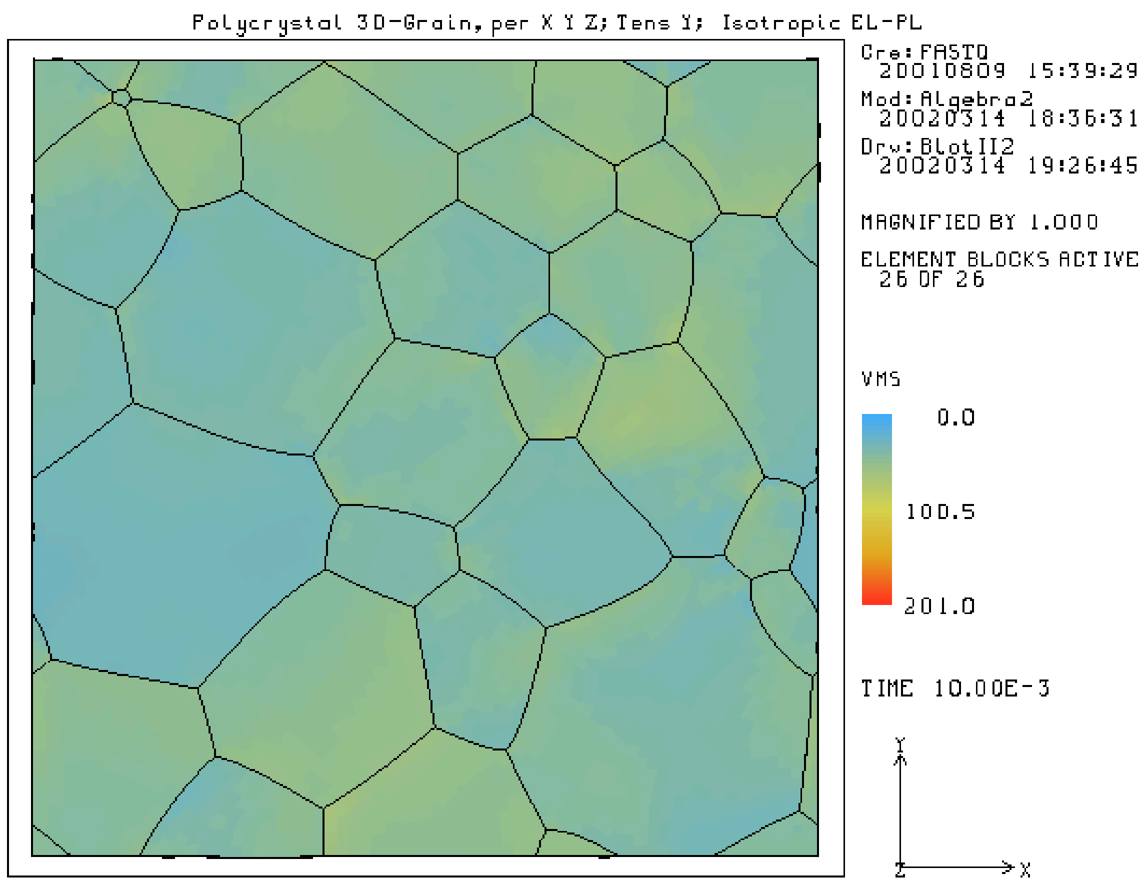
- Perform tensile hold test: Pull to 1% elongation, hold while grains grow.
- Interfacial, elastic, and plastic driving forces are included.
- Note stress concentrations at triple junctions and increasing internal stress.

<u>Inputs:</u>

C_{11} = 168.4 MPa
C_{12} = 121.4 MPa
C_{44} = 75.4 MPa
τ_o = 168.4 MPa
A = 121.4 MPa
n = 75.4 MPa

<u>Output:</u>

von Mises Stress [MPa]



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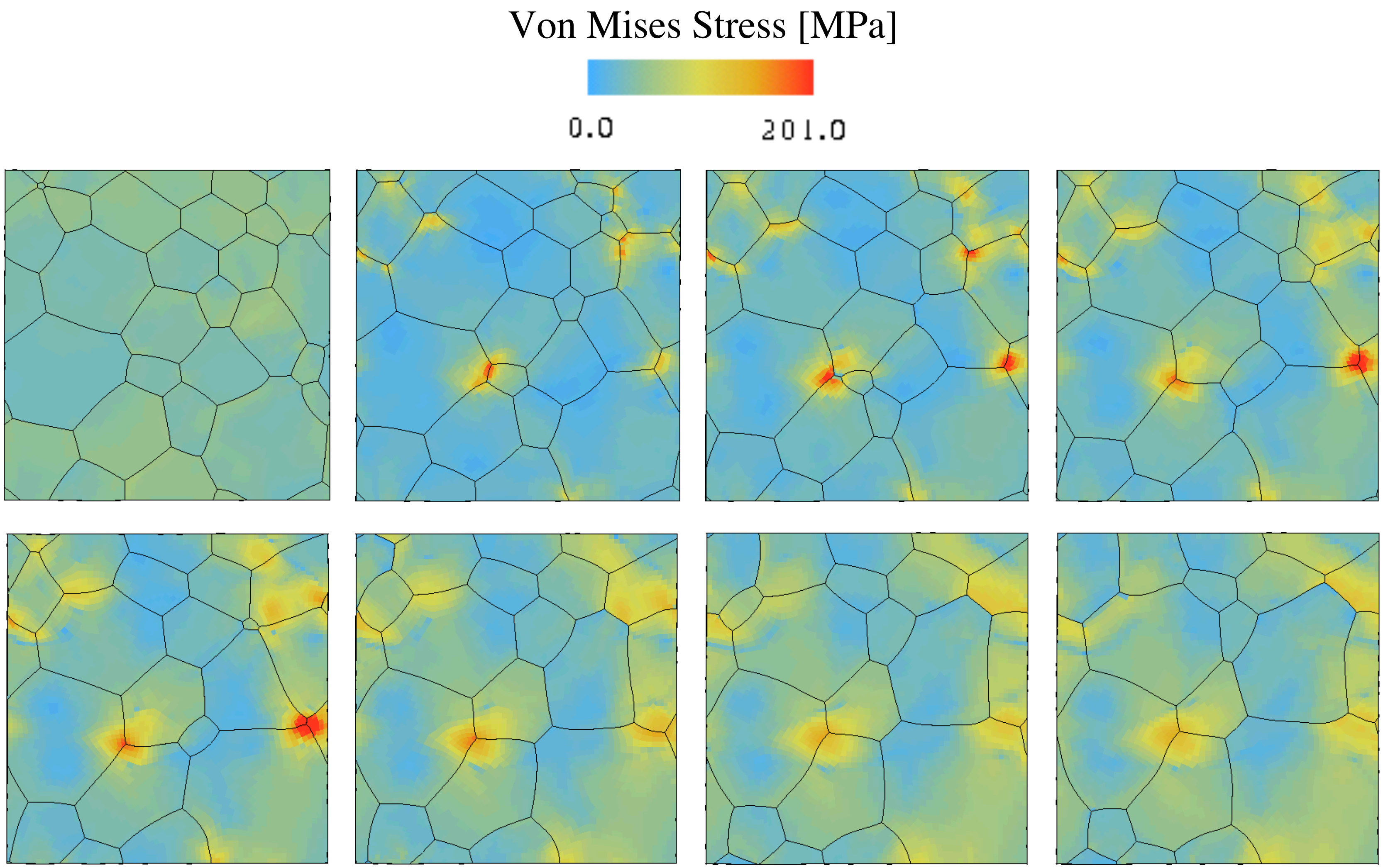
Grain growth and stress evolution in 1% tensile hold test



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Dislocation density evolution in 1% tensile hold test

- Pull to 1% elongation, hold while grains grow.
- Dislocations are swept out by moving boundaries.
- Dislocation density increases at triple junctions.

<u>Inputs:</u>

C_{11} = 168.4 MPa

C_{12} = 121.4 MPa

C_{44} = 75.4 MPa

τ_o = 168.4 MPa

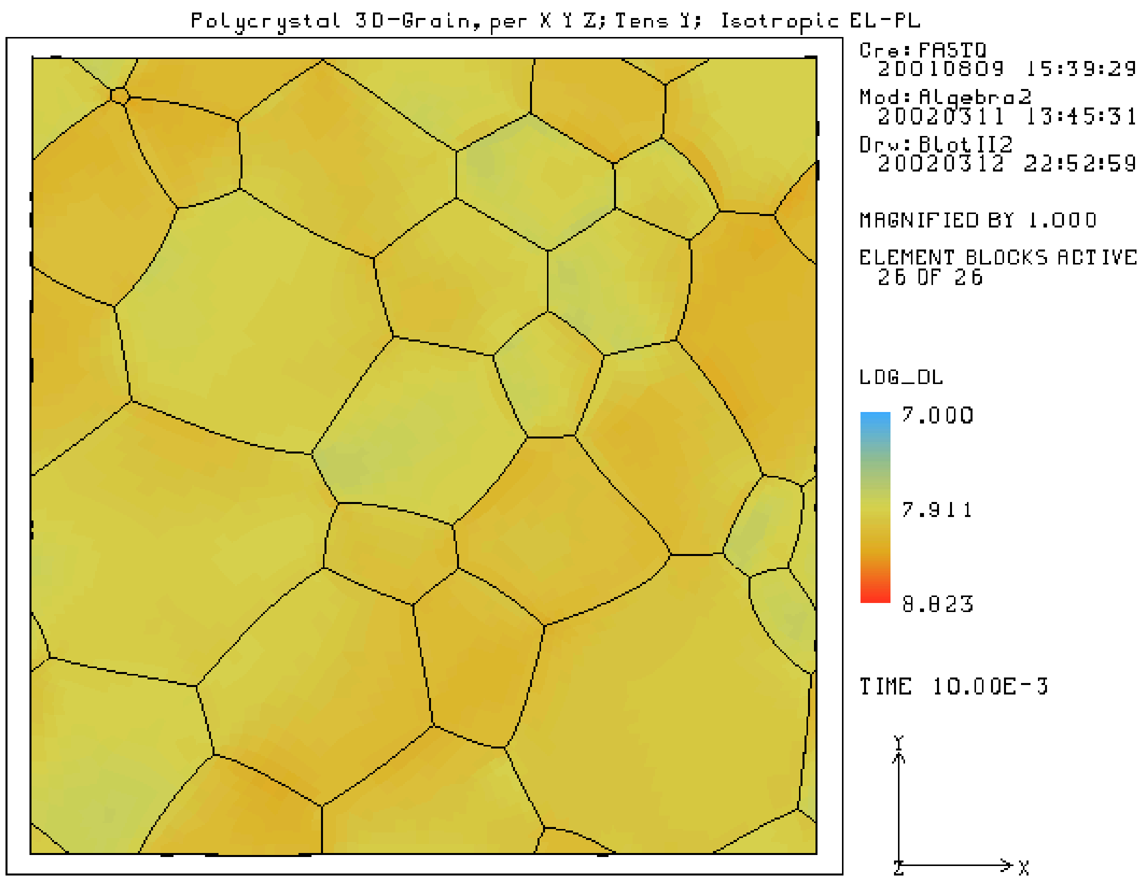
A = 121.4 MPa

n = 75.4 MPa

<u>Output:</u>

$\log(\rho_\perp)$

$$\rho_\perp = \left(\frac{\tau_{crss} - \tau_o}{\alpha G b} \right)^2 \quad [\mathrm{cm}^{-2}]$$



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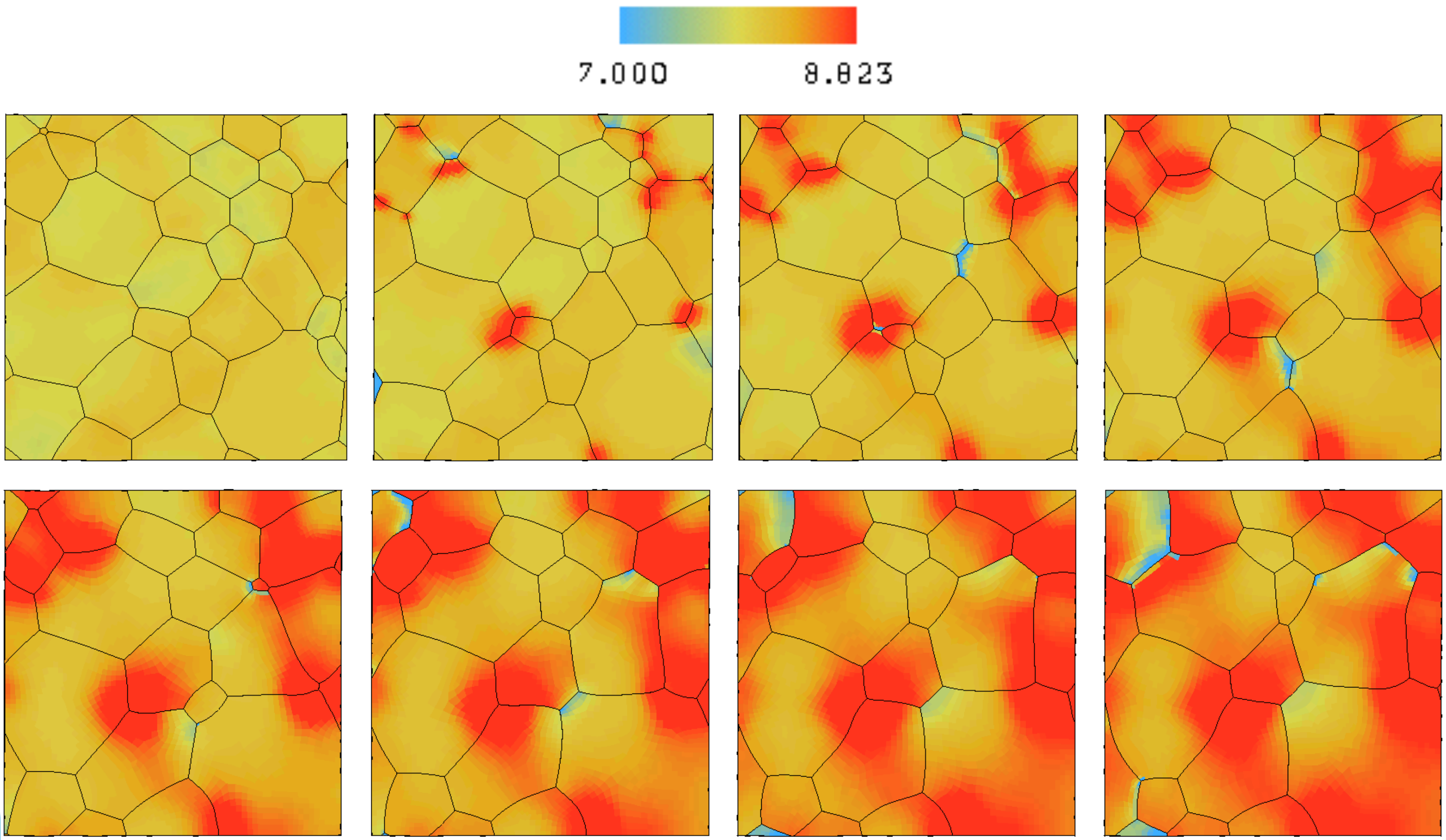
Dislocation density evolution in 1% tensile hold test

$$\log(\rho_{\perp}) \qquad \rho_{\perp} = \left(\frac{\tau_{crss} - \tau_o}{\alpha G b}\right)^2 \qquad [\mathrm{cm}^{-2}]$$



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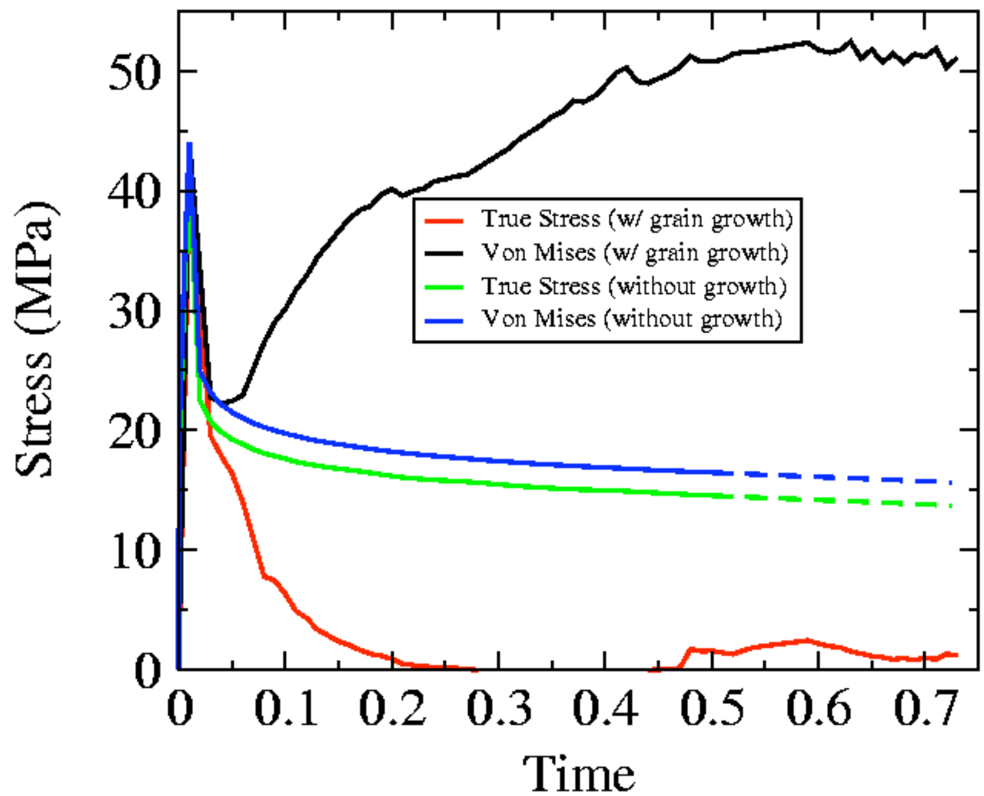
Stress evolution during 1% tensile hold test

- Load drops during grain growth, but internal stresses rise.
- This effect is directly attributable to the actions and interactions of evolving grains.
- Traditional continuum models do not exhibit this behavior.

⇒The power of microstructural modeling is revealing the effects of the discrete microstructural network.



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Conclusion

- To capture the link between microstructure and plasticity, we have directly coupled the evolution of microstructure and micromechanics.
- Microstructure and micromechanics are interdependent; both are required for a full representation of materials response.

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