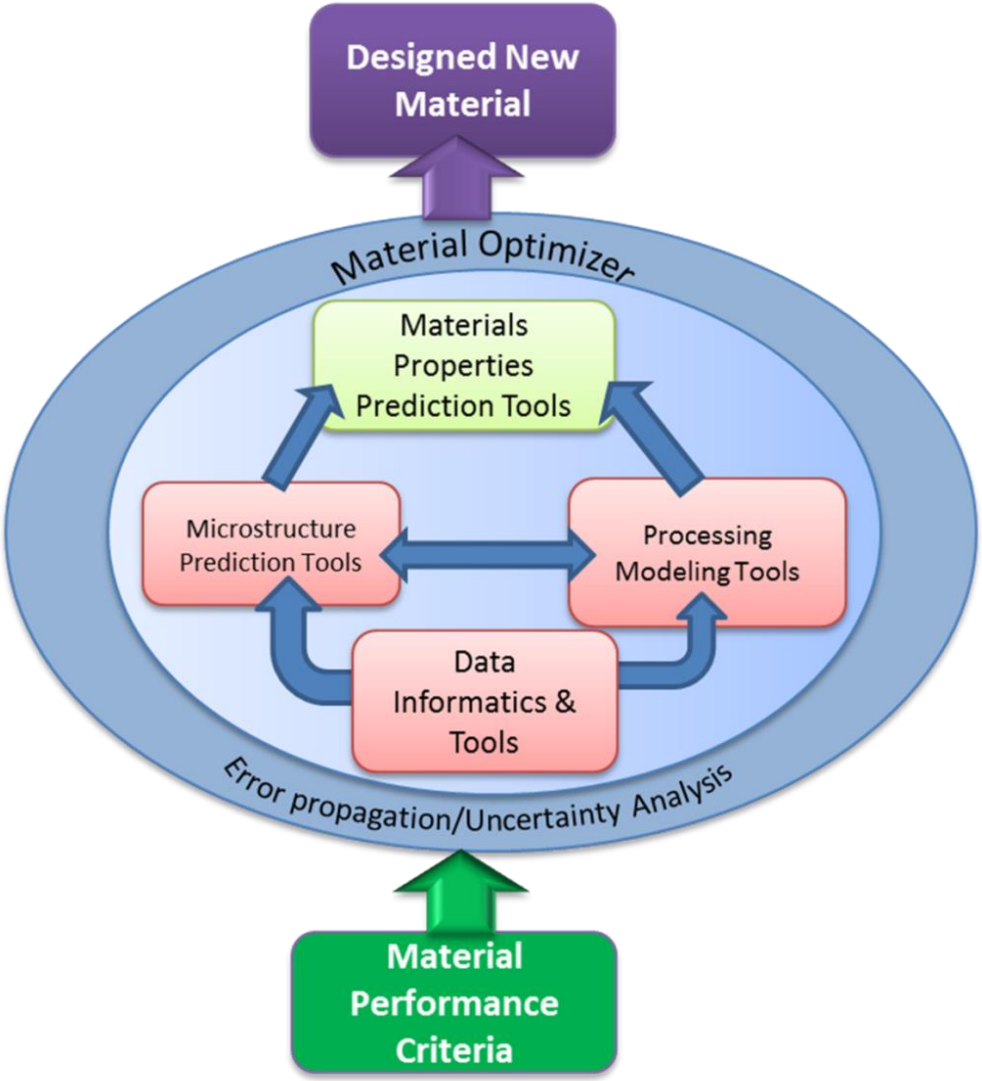
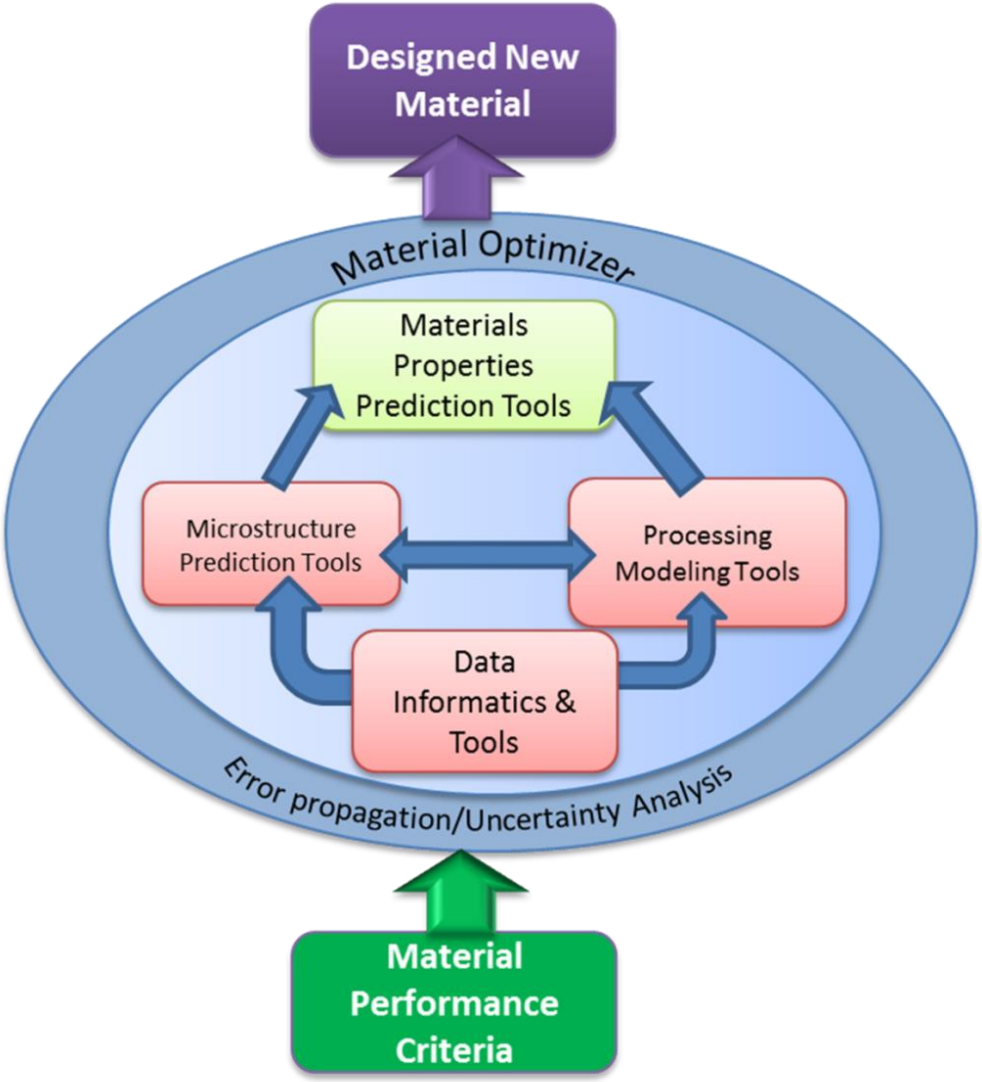
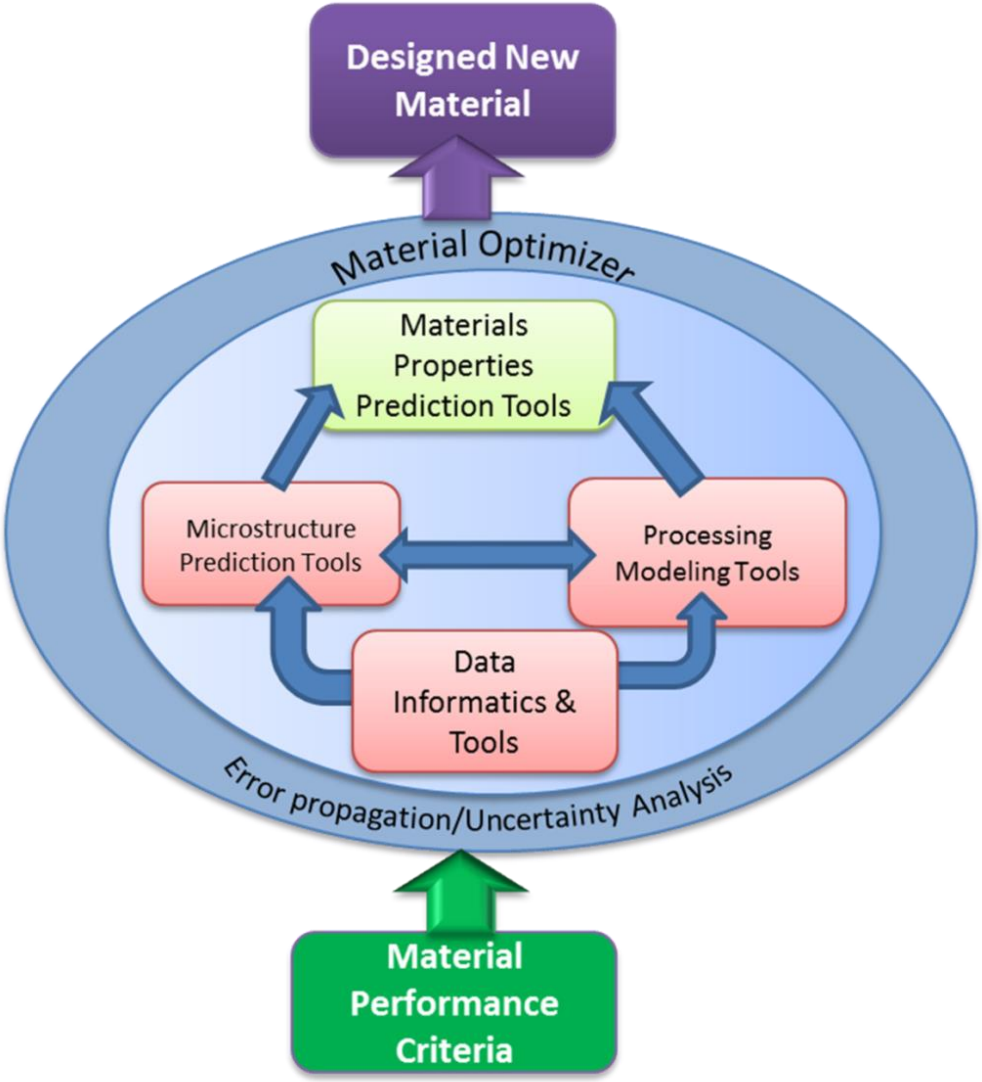

Designed New Material
Material Optimizer
Materials Properties Prediction Tools
Microstructure Prediction Tools
Processing Modeling Tools
Data Informatics & Tools
Error propagation/Uncertainty Analysis
Material Performance Criteria

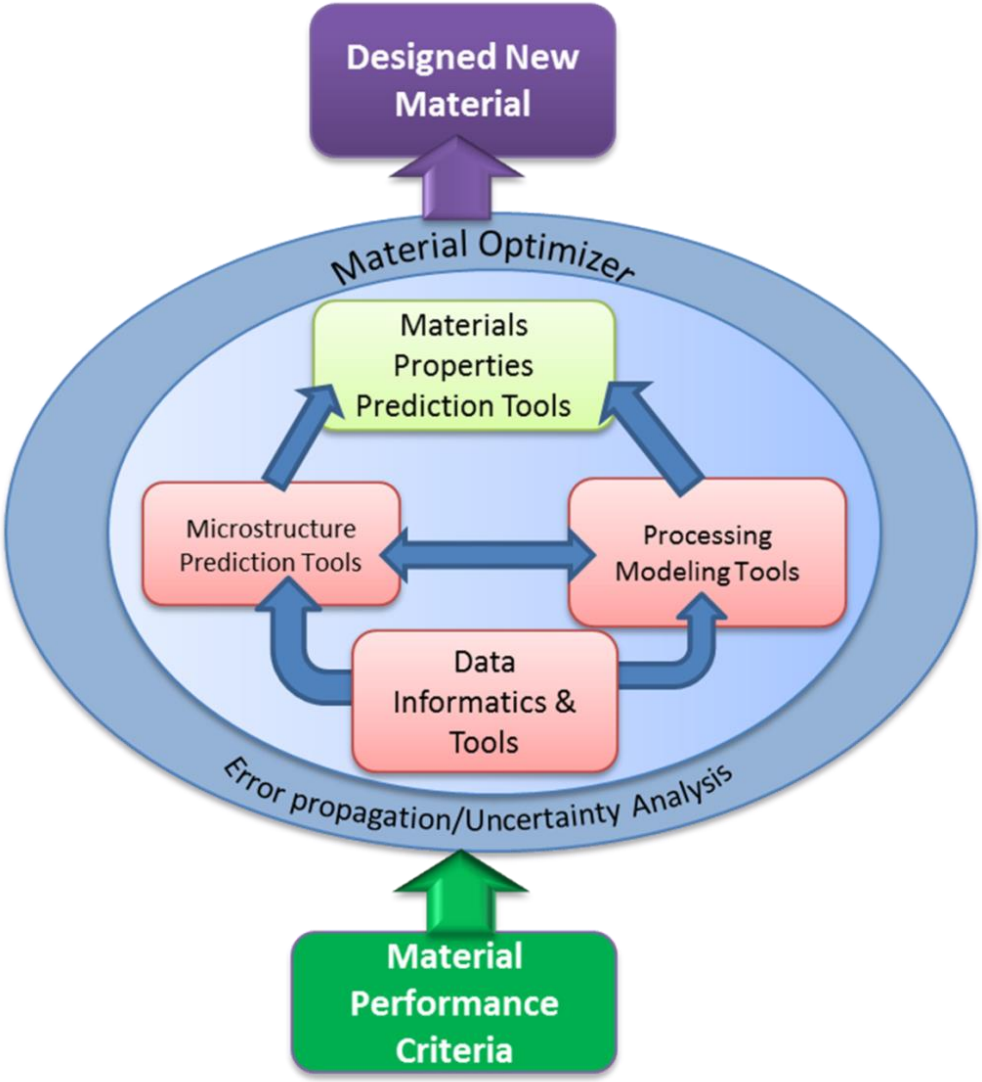


Requirements



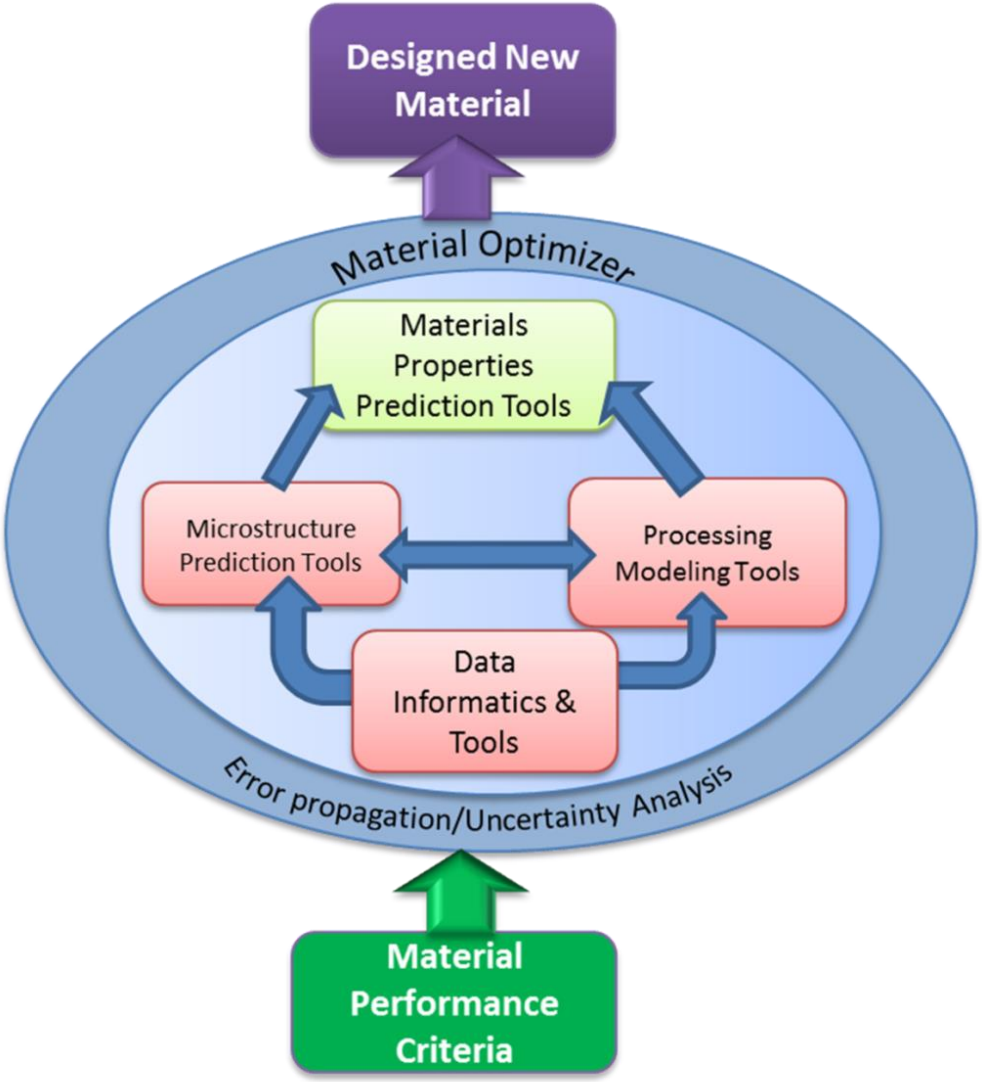
Requirements

1. “DATA”



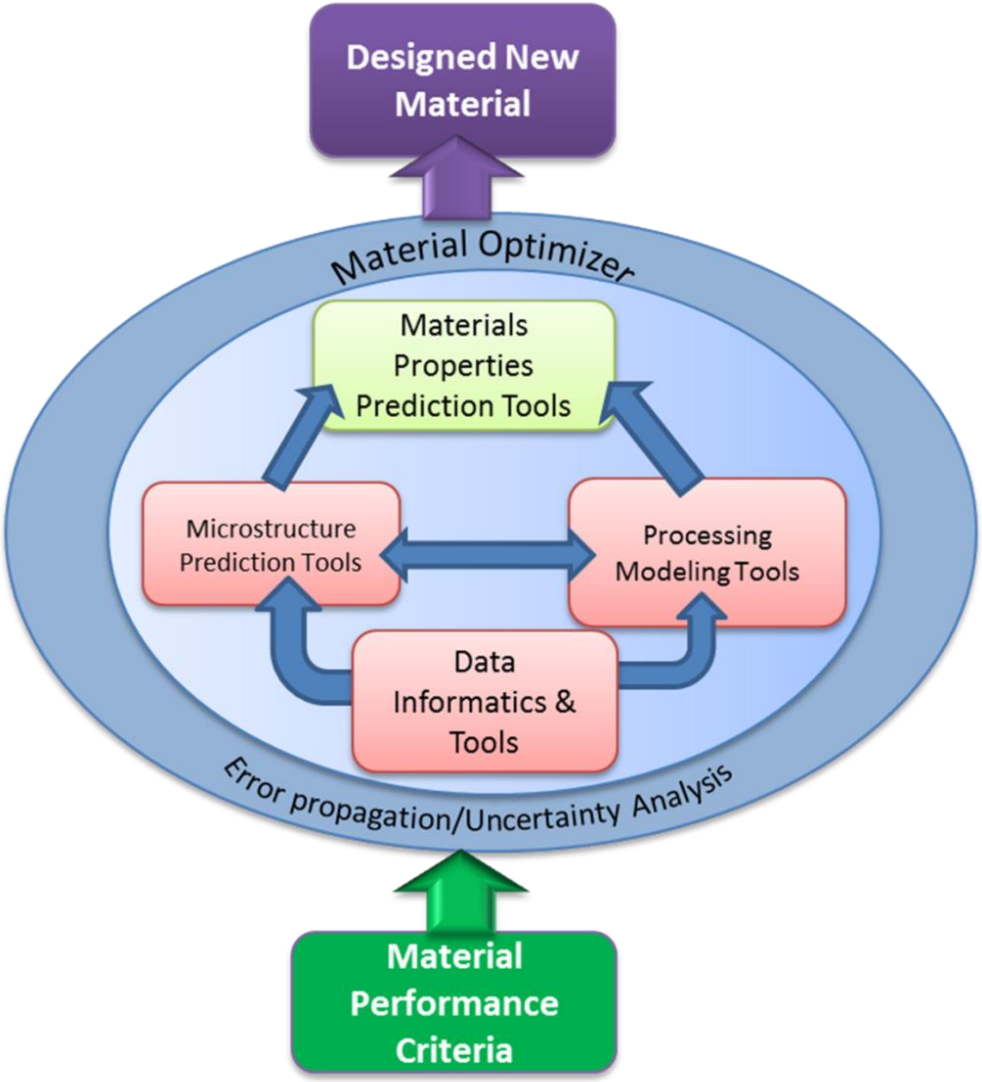
Requirements

1. "DATA"
2. Interdisciplinary tools



Requirements

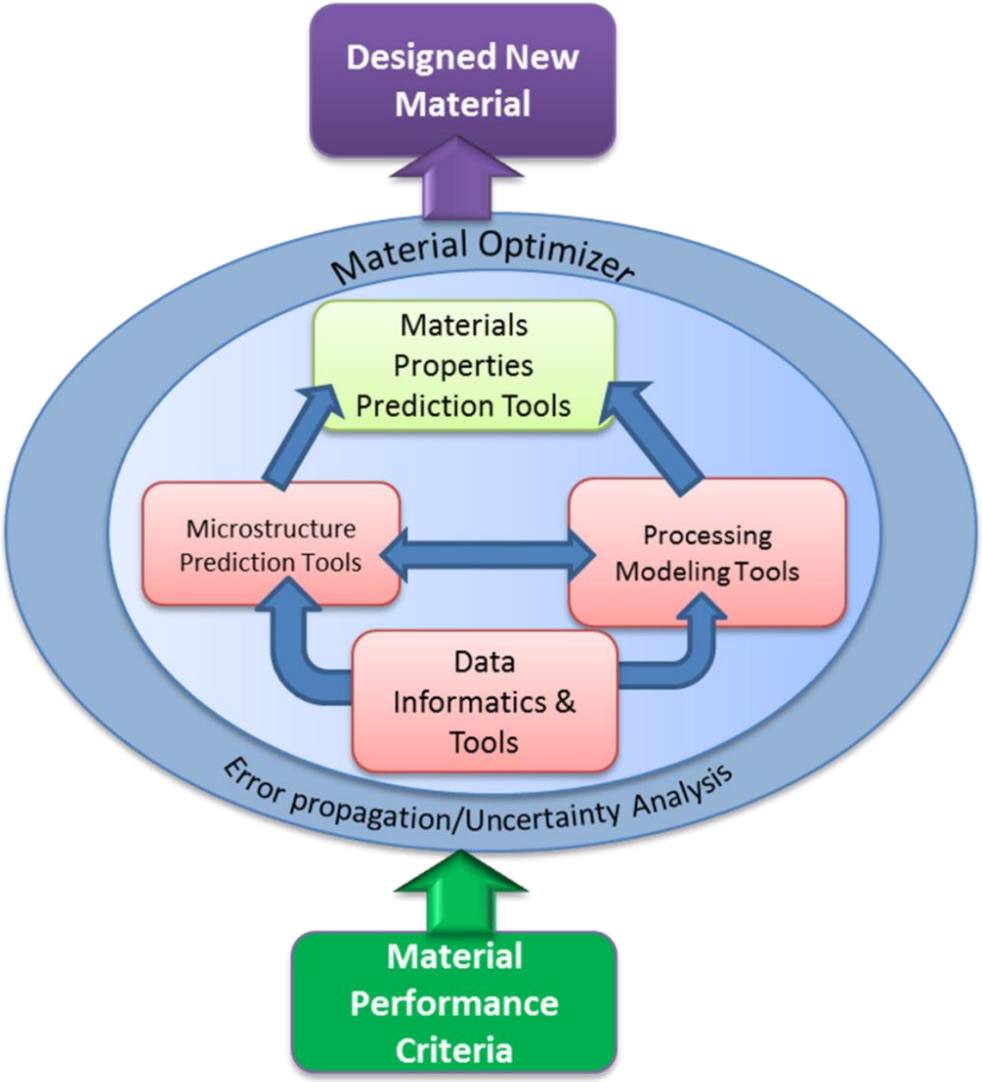
1. "DATA"
2. Interdisciplinary tools
3. Effective optimizer



Requirements

1. "DATA"
2. Interdisciplinary tools
3. Effective optimizer

Demands

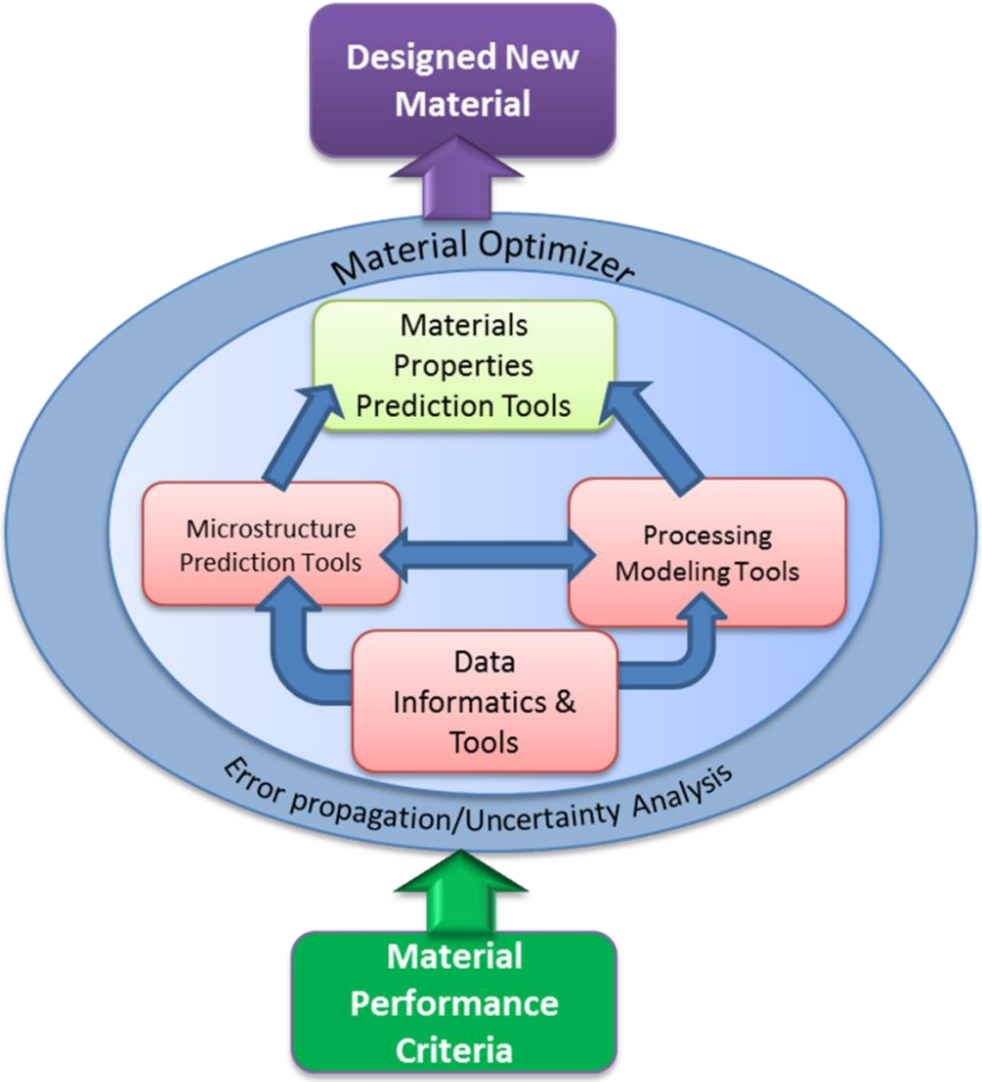


Requirements

1. "DATA"
2. Interdisciplinary tools
3. Effective optimizer

Demands

1. Low computational cost



Requirements

1. "DATA"
2. Interdisciplinary tools
3. Effective optimizer

Demands

1. Low computational cost
2. Easy model-switching

A computational framework for designing Ni-based superalloy

S. Li, U. Kattner, C. Campbell,
D. Wheeler, A. Reid

National Institute of Standards and Technology

May. 14 2015

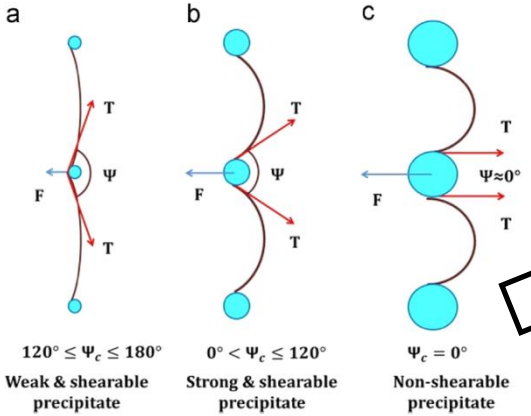
Outline

- ❖ Background: $\gamma - \gamma'$ Ni Base Superalloy
- ❖ Computational Framework
  - Classical Nucleation, Growth and Coarsening Models
  - Elastic Deformation: Statistical tool, PyMKS
  - Plastic Deformation: Kocks-Mecking & energy conservation models
  - Optimization
- ❖ Summary

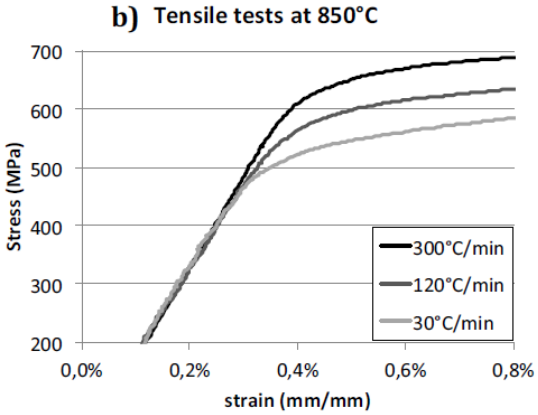
$\gamma - \gamma'$ Ni-Base Superalloy

Olson, 1997
Ahmadi et al., 2014
Le Baillif et al., 2014

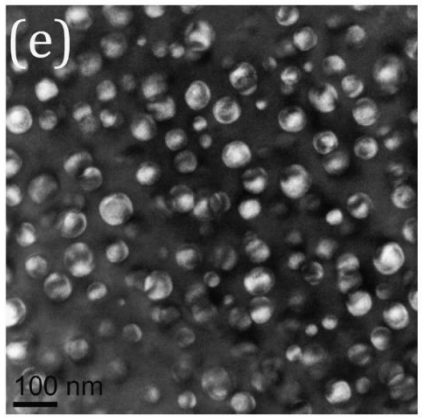
- γ and γ' microstructure
- γ' strengthening
- Chemistry & geometry properties affect performance
- Optimum composition & processing conditions are required



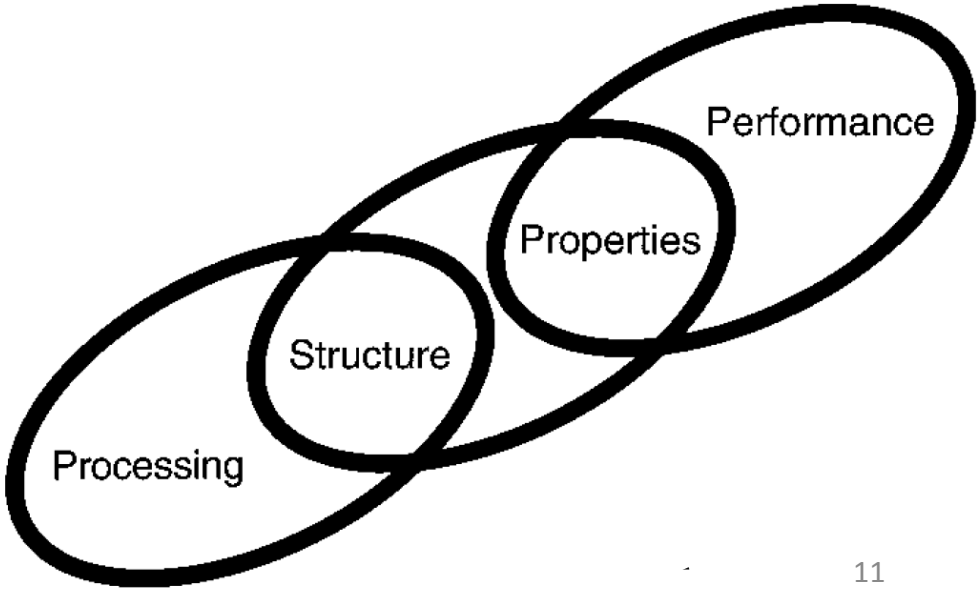
Precipitation hardening

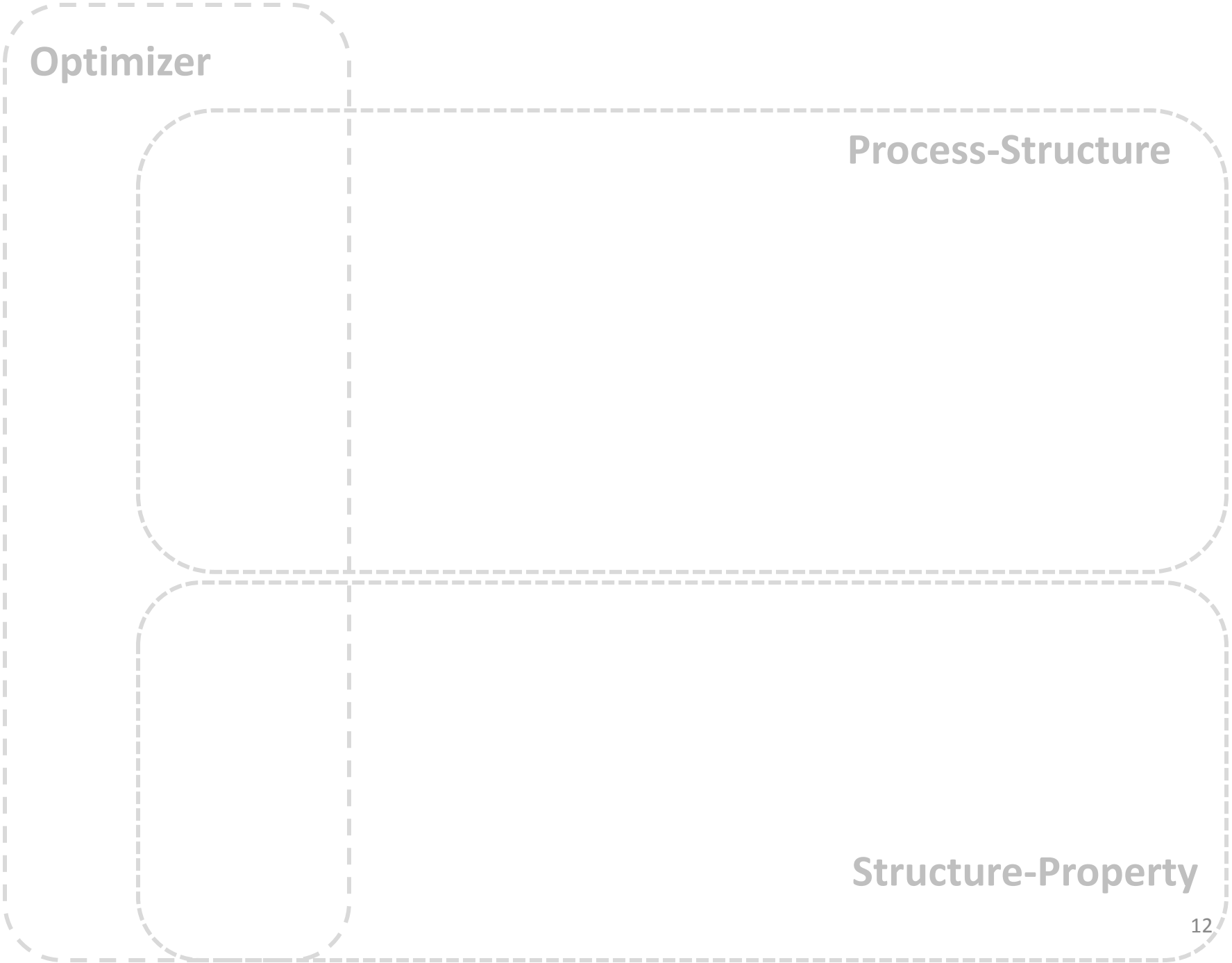


High Temperature Application



γ/γ' Microstructure



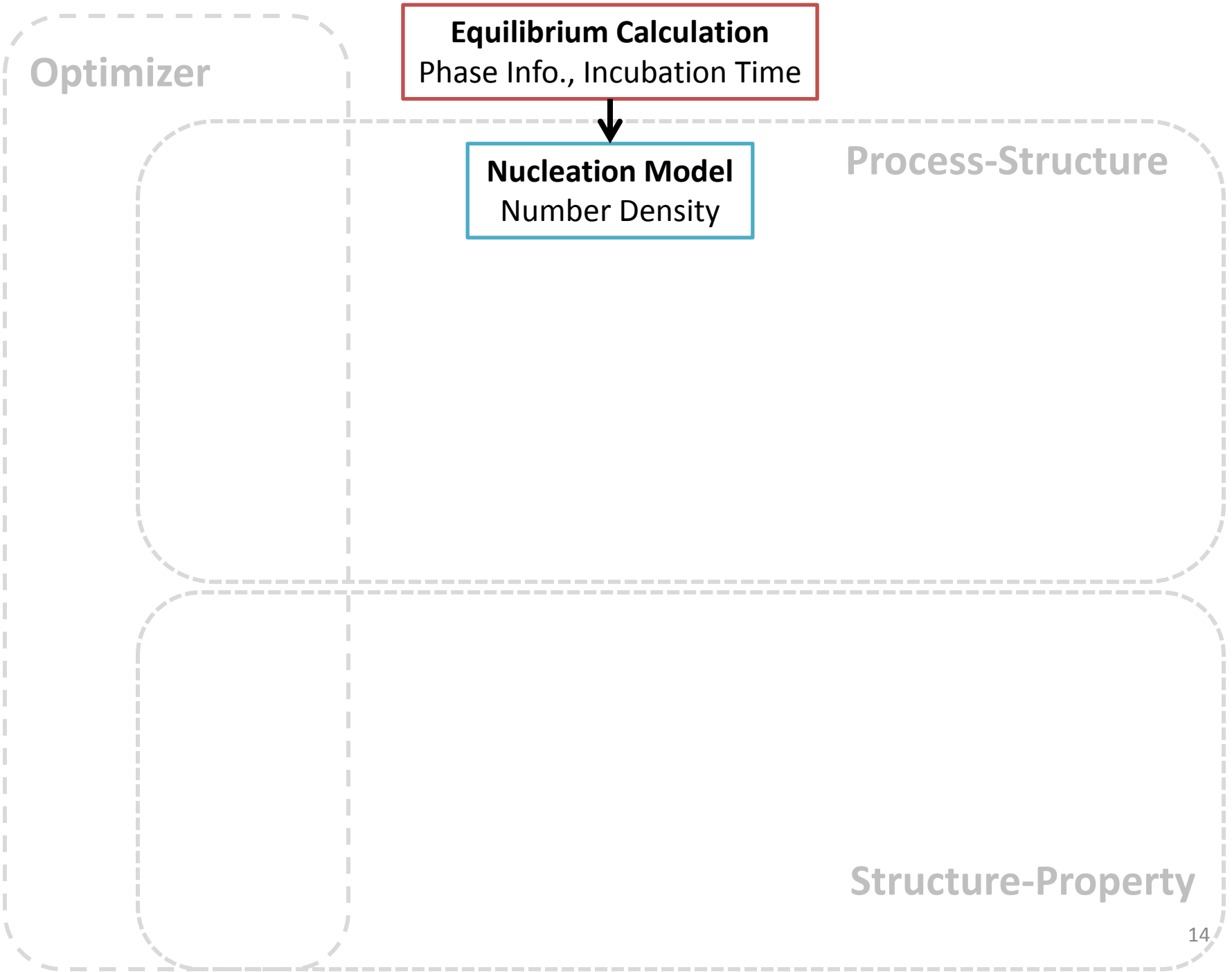

Optimizer
Process-Structure
Structure-Property

Optimizer

Equilibrium Calculation
Phase Info., Incubation Time

Process-Structure

Structure-Property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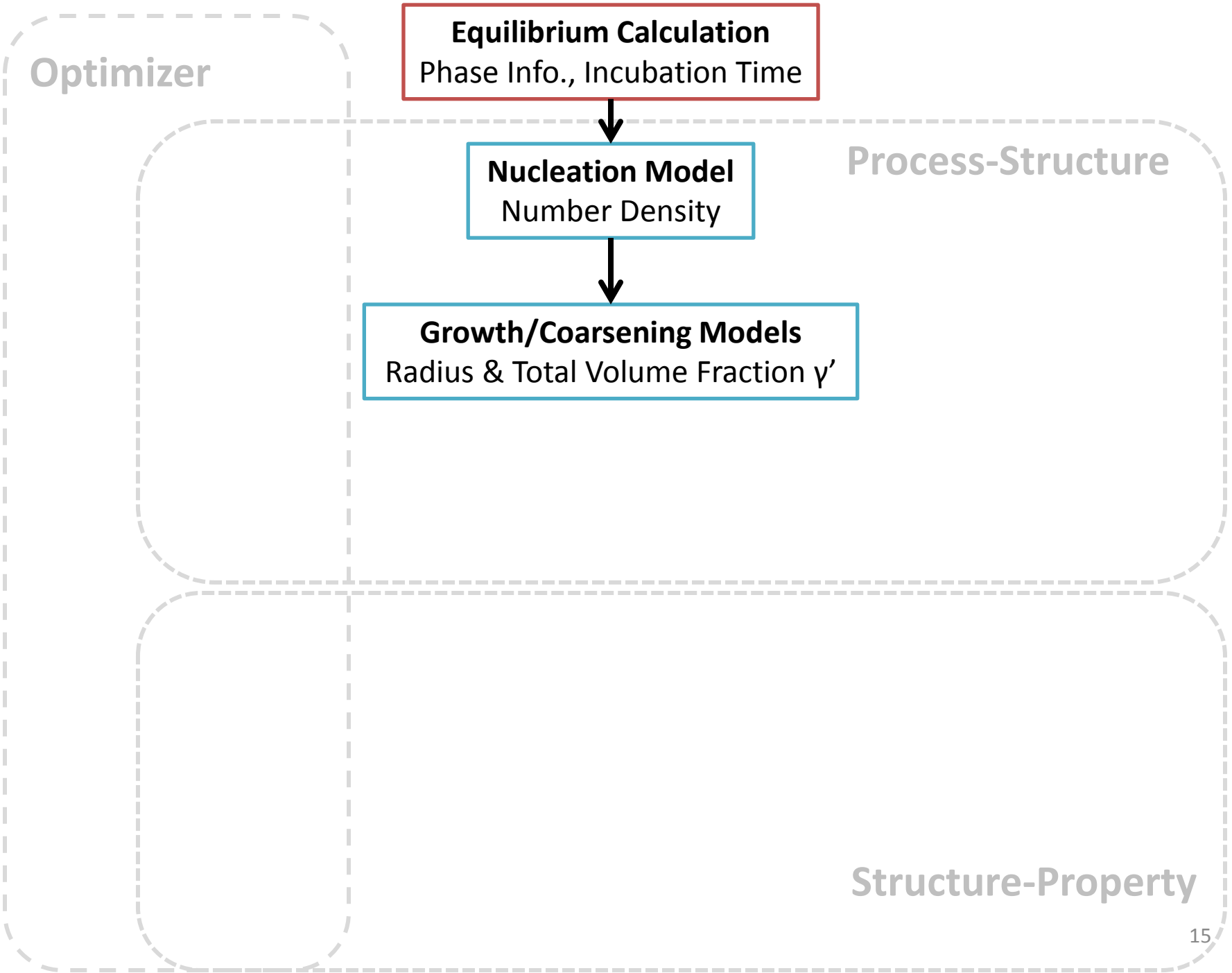
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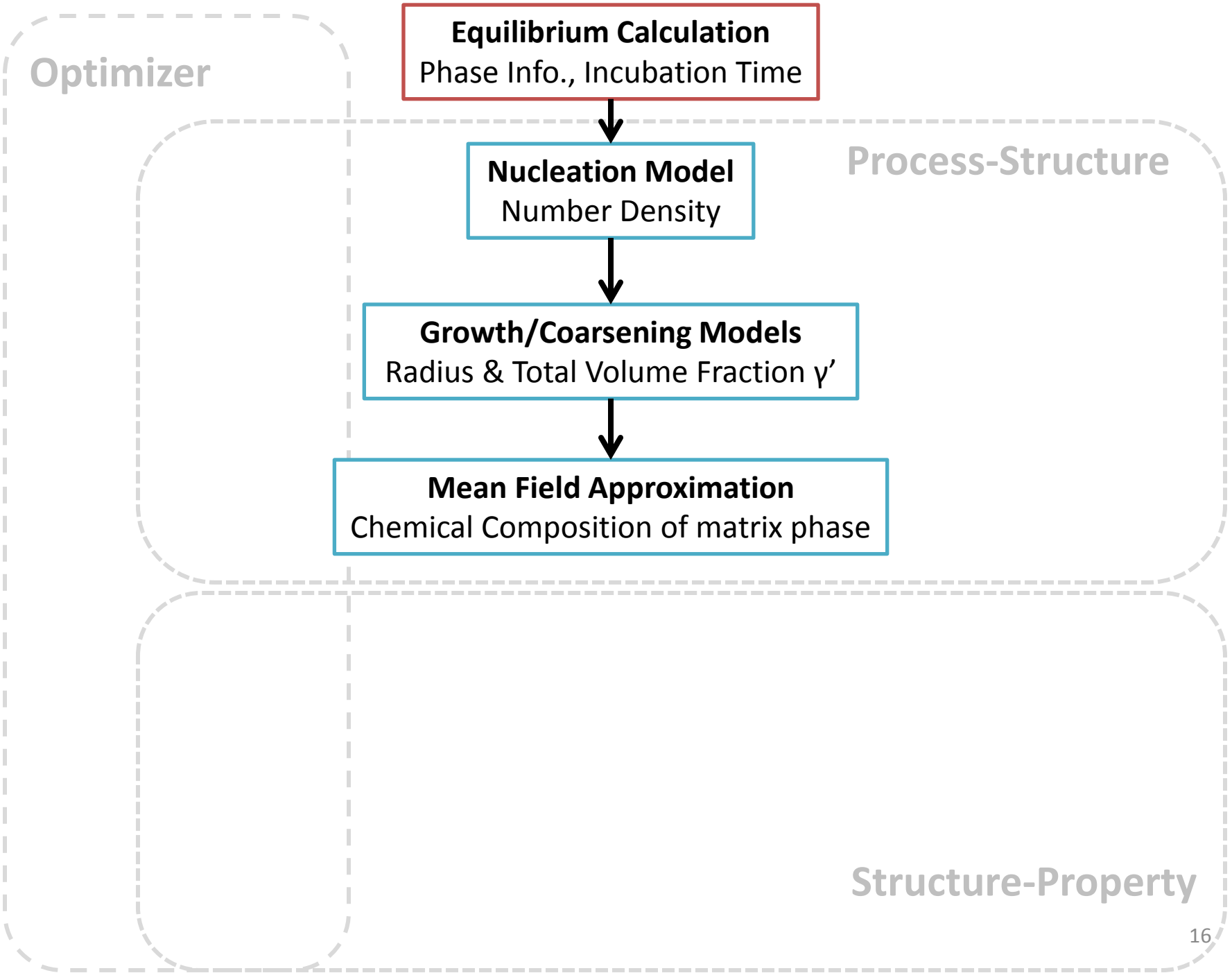
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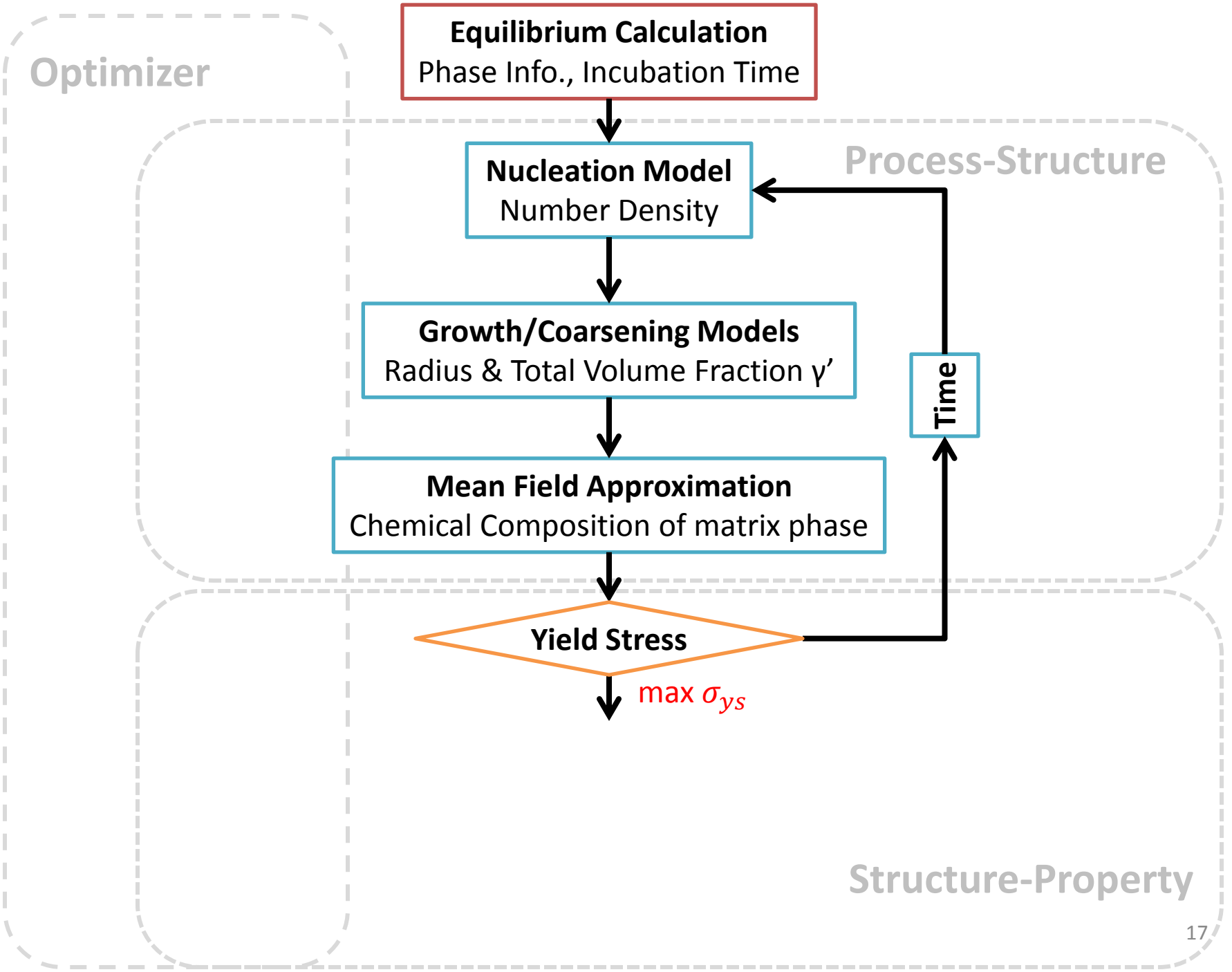
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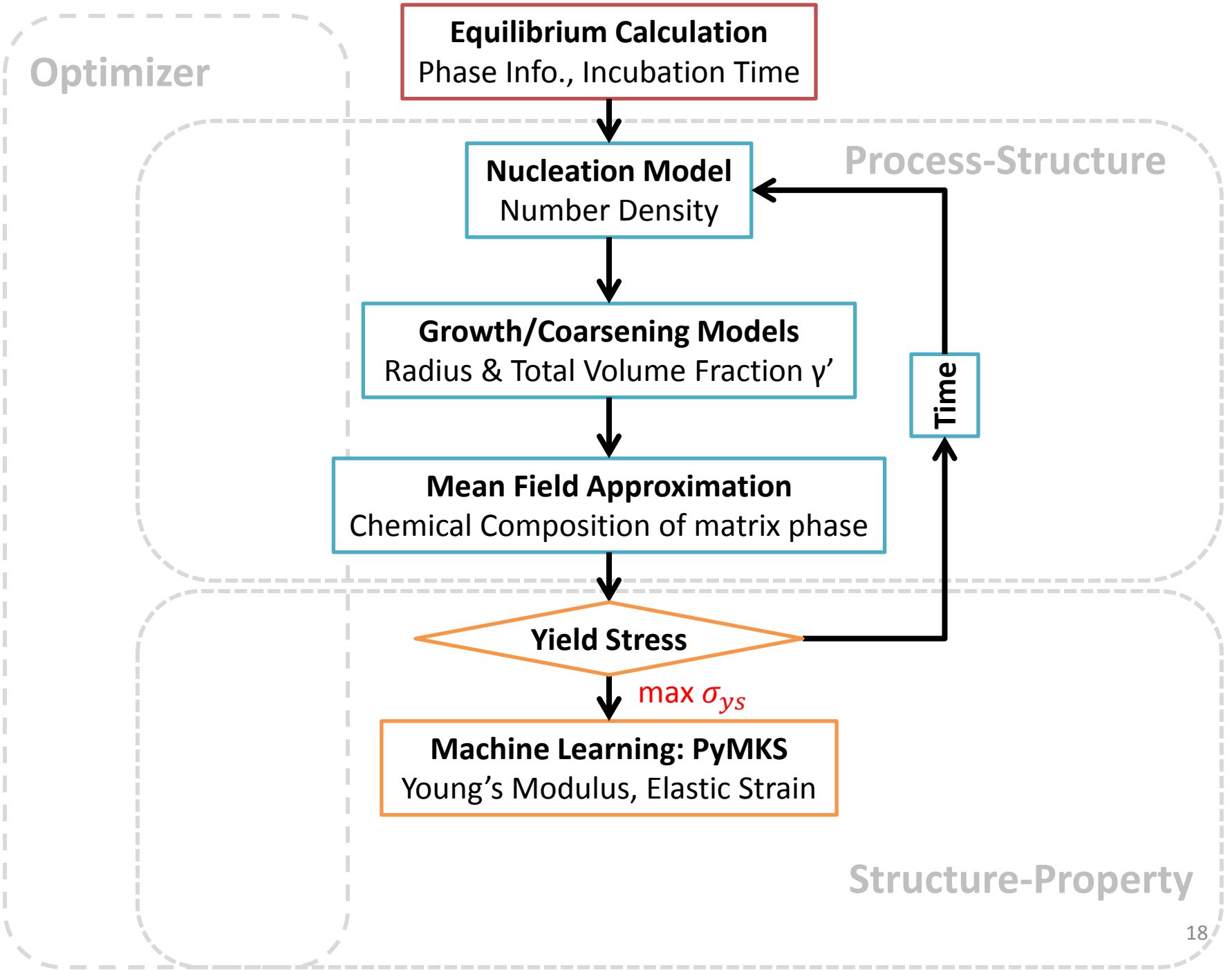
max σ_{ys}
Structure-Property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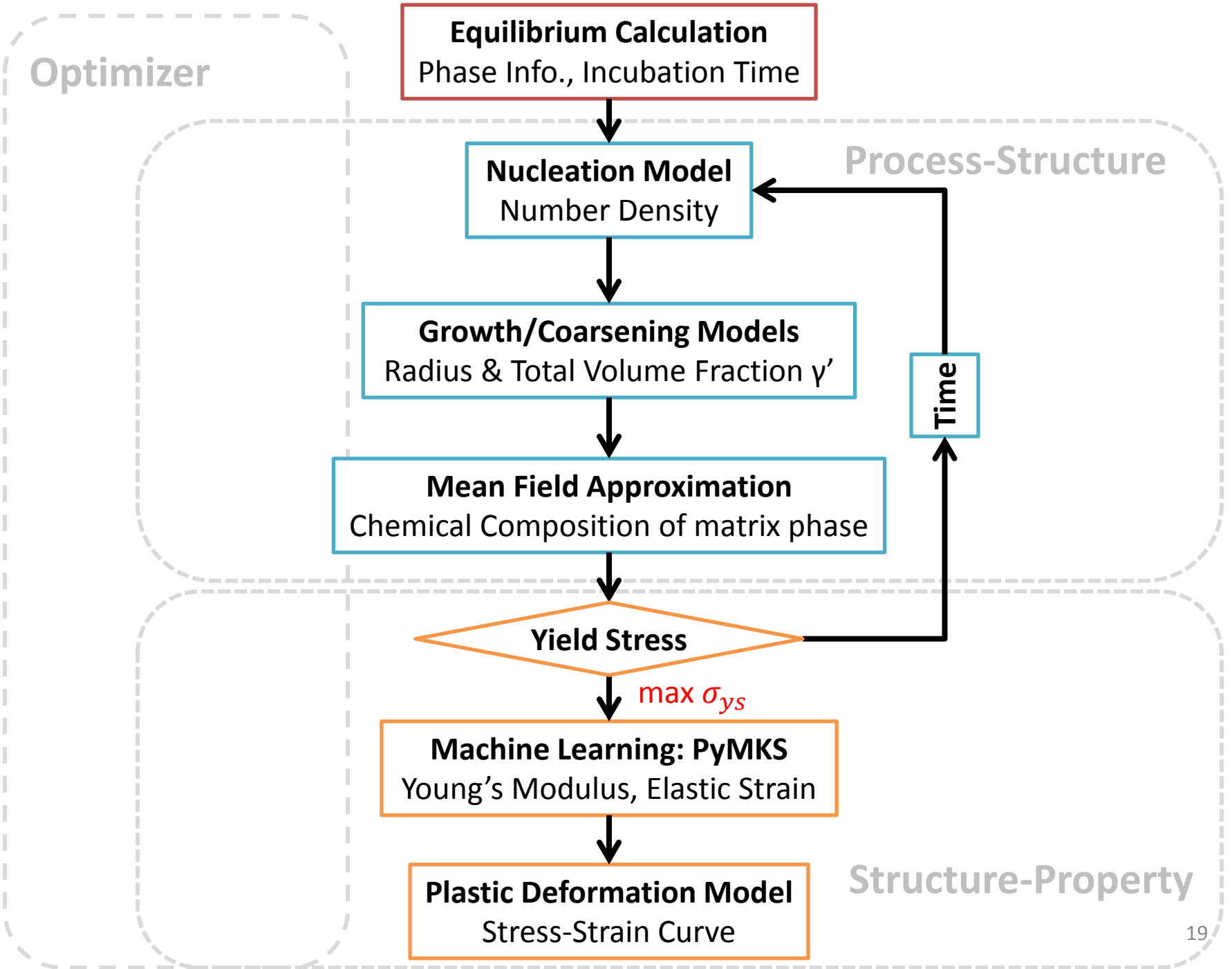
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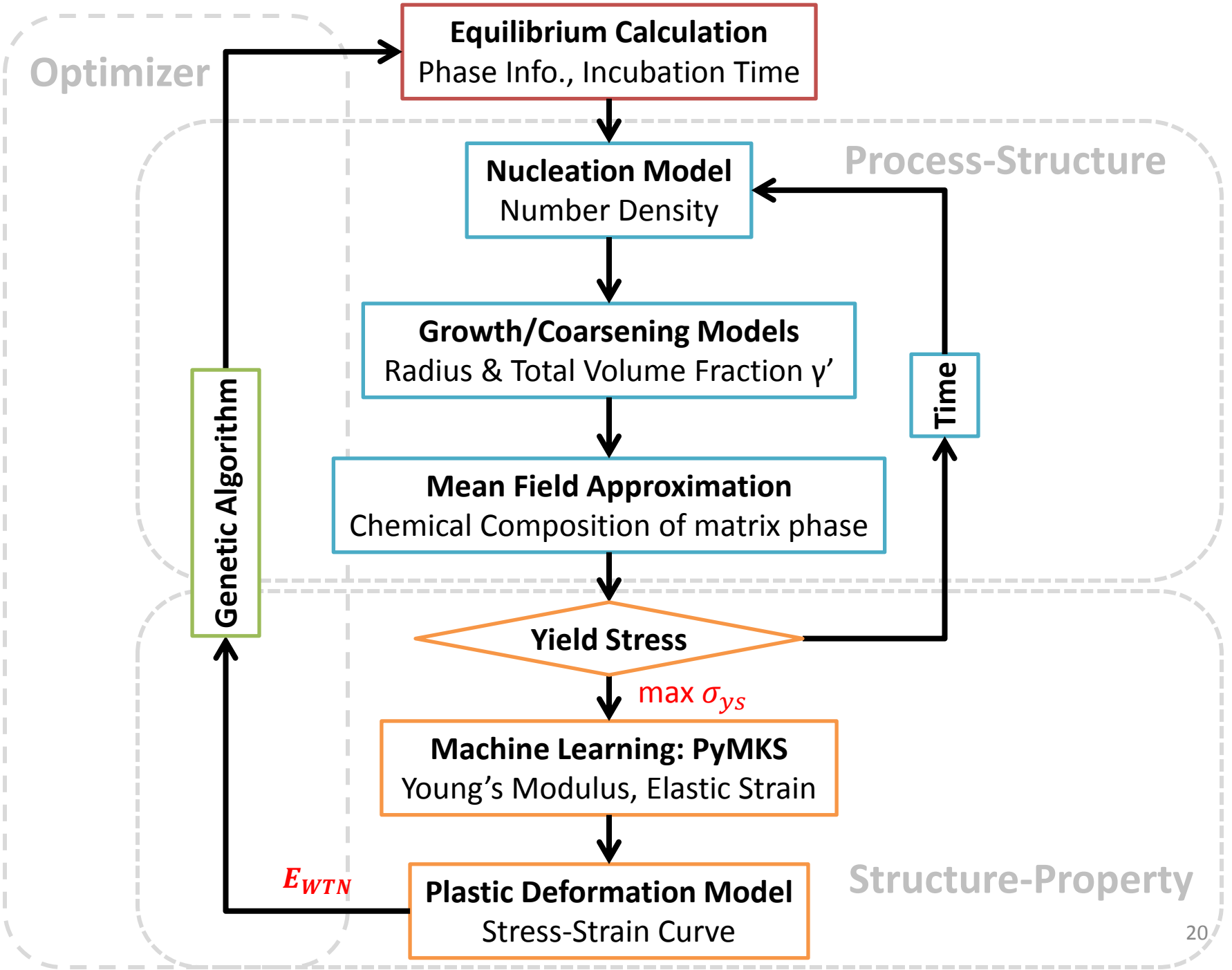
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Homogeneous, NON-Steady-State Nucleation

Russell, 1978
Wagner et al., 2001

$$\dot{N}(t) = Z\beta N_0 \exp\left(\frac{-\Delta G^*}{K_B T}\right) \exp\left(\frac{-\tau}{t}\right)$$

- Cluster size is estimated by Boltzmann distribution of total number of clusters, N_0
- Interface energy (E_{INT}) and N_0 are the remaining parameters
- β - rate of atom jumps from matrix to precipitate
- Zeldovich factor, Z, is employed to correct the equation
- The parameters are calculated using Thermo-Calc with TCNI6 database

$$\Delta G^* = \frac{16\pi}{3}\frac{E_{INT}^3}{\Delta G_N^2}$$

$$\Delta G_N = \frac{\Delta G_{ch}}{V_m^{\gamma'}} = -\frac{RT}{V_m^{\gamma'}}\sum_i \bar{C}_i^{\gamma'} \ln\frac{a_i}{\bar{a}_i^{\gamma}}$$

$$Z = \frac{V_M^{\beta}}{2\pi N_A r_0^2}\sqrt{\frac{E_{INT}}{K_B T}}$$

$$\beta = \frac{4\pi r_0^2}{a^4}\left[\sum \frac{\left(\bar{C}_i^{\gamma'} - \bar{C}_i^{\gamma}\right)^2}{\bar{C}_i^{\alpha} D_i}\right]^{-1}$$

$$r_0 = -\frac{2E_{INT}V_M^{\beta}}{\Delta G_N}$$

$$\tau = \frac{1}{\theta Z^2 \beta}$$

Growth & Coarsening

Rougier et al., 2013
Perez et al., 2008

γ' growth

$$\frac{dR}{dt} = \frac{D_i^{\gamma}}{\left[1 - \lambda_j \sqrt{\pi} \exp\left(\lambda_j^2\right) \mathrm{erfc}\left(\lambda_j\right)\right] R} \frac{C_i^{\gamma} - \bar{C}_i^{\gamma}}{\left(\bar{C}_i^{\gamma'} - \bar{C}_i^{\gamma}\right)}$$

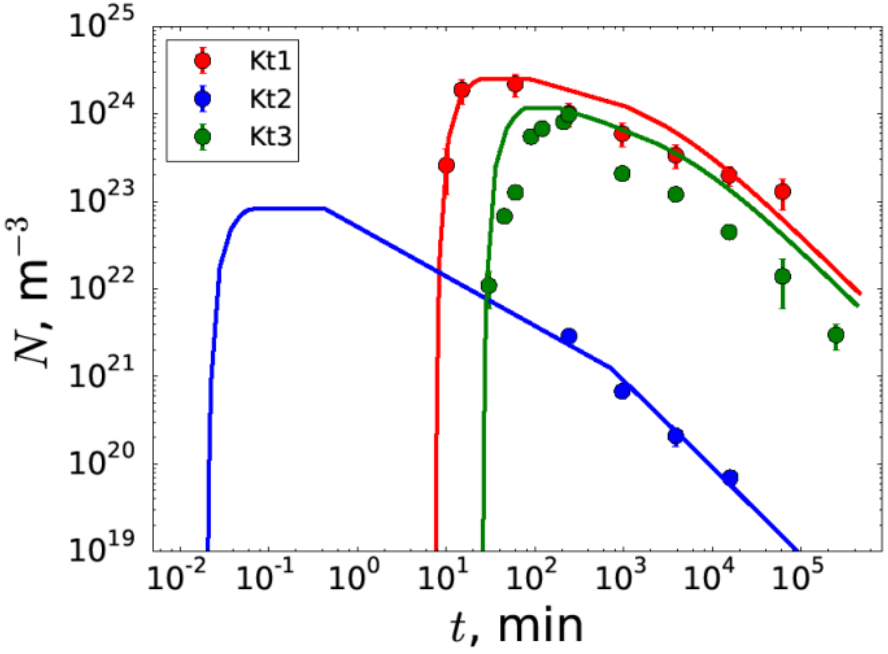
- $\bar{C}_i^{\gamma'}$ is taken as the equilibrium composition in γ'
- $\left[1 - \lambda_j \sqrt{\pi} \exp\left(\lambda_j^2\right) \mathrm{erfc}\left(\lambda_j\right)\right] R$ stands the Effective Diffusion Distance

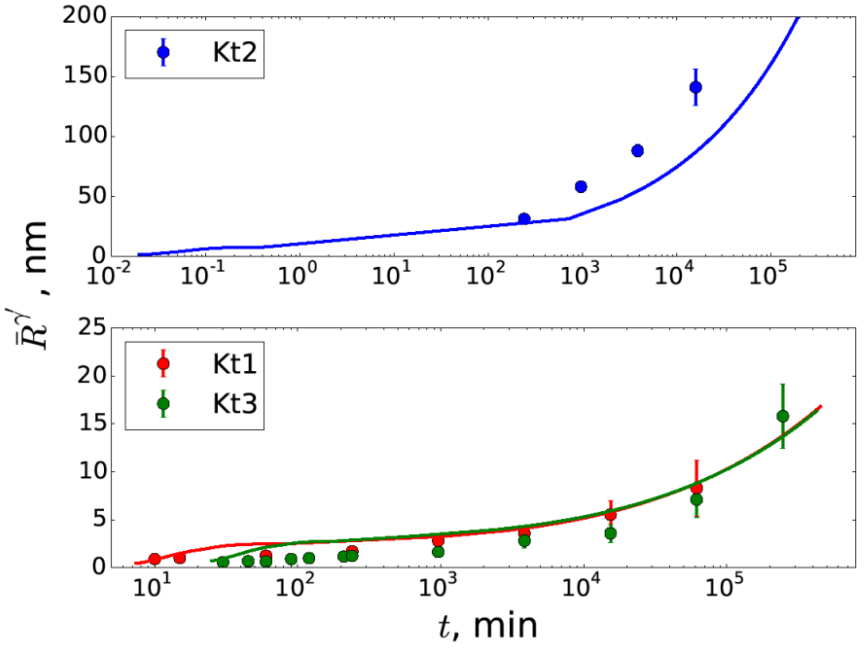
γ' coarsening

$$\frac{dR}{dt} = \frac{8}{27} \frac{E_{INT} V_M^{\gamma'}}{R^2 N_A k_B T} \frac{D_i^{\gamma} \bar{C}_i^{\gamma}}{\bar{C}_i^{\gamma'} - \bar{C}_i^{\gamma}}$$

Determine E_{INT} and N_0

	Experimental			Data Regression	
	Composition, %	T_p, K	reference	E_{int}, mJ/m^2	N_0, 1/m^2
Kt1	Ni-7.5Al-8.5Cr	873	Booth-Morrison et al., 2008	15	1.5x10^{26}
Kt2	Ni-9.8Al-8.3Cr	1073	Sudbrack et al., 2008	24	5x10^{27}
Kt3	Ni-6.5Al-9.5Cr	873	Booth-Morrison et al., 2010	18	**4.0x10^{26}**





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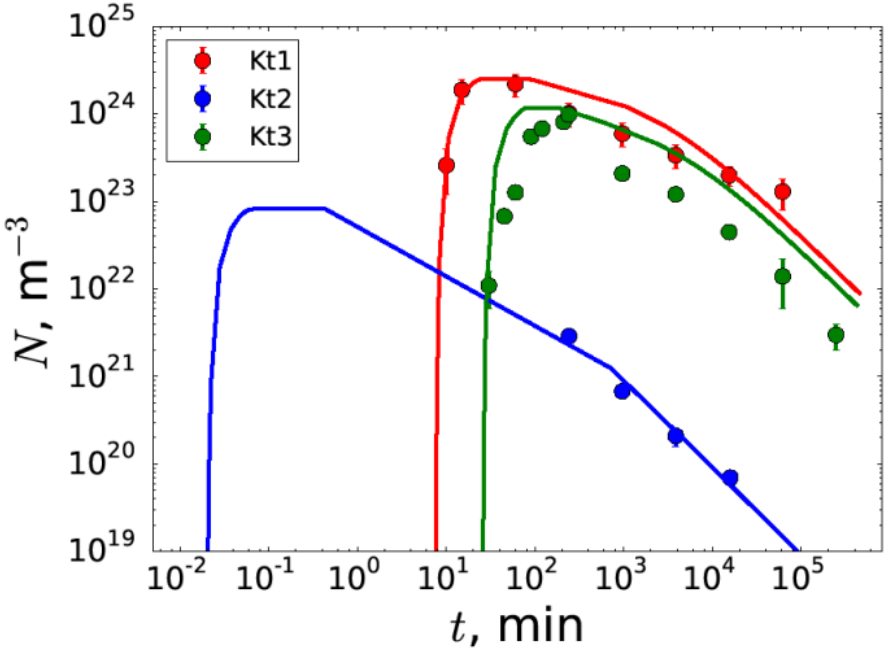
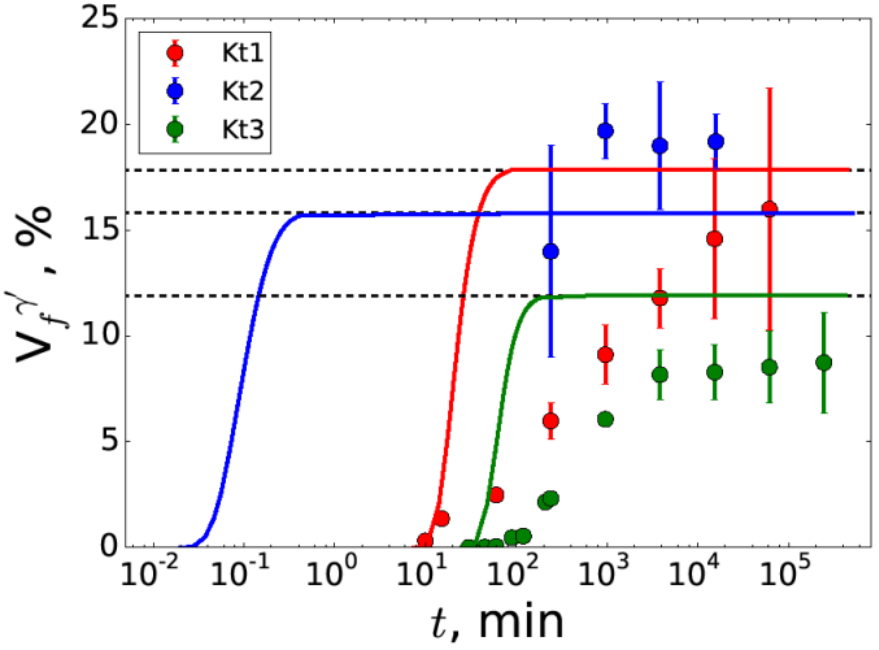




Determine E_{INT}

Nishizawa et al., 2001
Li et al., 2002

Nishizawa et al., 2001

$$E_{int} = \alpha|\Delta H^{\gamma\rightarrow\gamma'}|$$

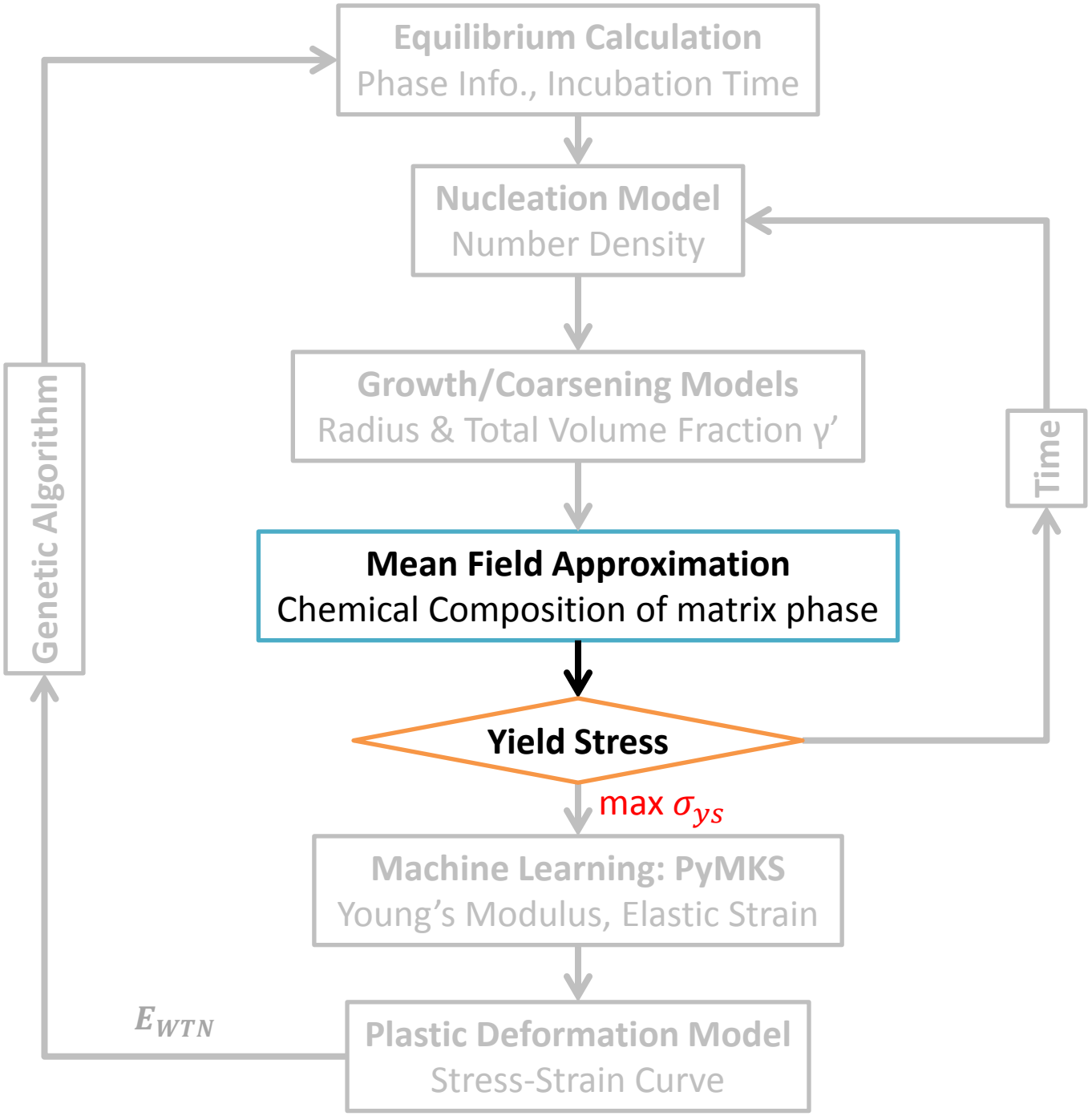
$\boldsymbol{E_{int}}$ & $|\Delta H^{\gamma\rightarrow\gamma'}|$

$\alpha = f(T_p)$

$\alpha = (3.75 \times 10^{-2} T_p - 2.23) \times 10^{-6}$

	Experimental		Computation	Parameter		
	Composition %	$\boldsymbol{T_p}$ Kelvin	$\lvert\Delta H^{\gamma\rightarrow\gamma'}\rvert$ 10^4 J/mol	$\boldsymbol{E_{int}}$ mJ/m^2	α 10^{-6} mol/m^2	$\boldsymbol{E_{int,cal}}$ mJ/m^2
Kt1	Ni-7.5Al-8.5Cr	873	1.52	15	0.99	15.
Kt2	Ni-9.8Al-8.3Cr	1073	1.34	24	1.80	24
Kt3	Ni-6.5Al-9.5Cr	873	1.64	18	1.10	17.1

$$E_{int} = (3.75 \times 10^{-2} T_p - 2.23) \times 10^{-6} |\Delta H^{\gamma\rightarrow\gamma'}|$$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Yield Stress

Thomas et al., 2006
Roth et al., 1997
Reed., 2006
Collins et al., 2014

$$\sigma_{YS} = \sigma_0 + \sigma_{SS} + \sigma_{H-P} + \sqrt{\sigma_{\rho,0}^2 + \boldsymbol{\sigma_p^2}}$$

- Calculations using results from previous steps: $Vf_{\gamma'}$, $r_{\gamma'}$, and composition of matrix
- Lattice friction (σ_0), solid solution (σ_{SS}) and Hall-Petch effect (σ_{H-P}) to yield stress is estimated [Roth97].
- σ_P follows the minimum value among σ_{wc} σ_{sc} and σ_{or}.
- E_{APB} is calculated

$$\sigma_{wc} = M\frac{\boldsymbol{E_{APB}}}{2b}\left[\left(\frac{6\bar{R}^{\gamma'}\boldsymbol{E_{APB}}V_f^{\gamma'}}{\pi L_T}\right)^{0.5} - V_f^{\gamma'}\right]$$

$$\sigma_{sc} = 0.22M\left(\frac{\mu b}{\bar{R}^{\gamma'}}\right)\left(\frac{\pi\bar{R}^{\gamma'}\boldsymbol{E_{APB}}V_f^{\gamma'}}{L_T} - V_f^{\gamma'}\right)^{0.5}$$

$$\sigma_{or} = M\frac{\mu b}{\bar{R}^{\gamma'}}\sqrt{\frac{V_f^{\gamma'}}{\pi}}$$

APB Energy

Miodownik et al, 1995

$$E_{APB,[111]} = \frac{W_1 - 3W_2 + 4W_3 \ldots}{\sqrt{3}\left(a^{\gamma'}\right)^2}$$

Atomic Bonding Energies

$$W_1 = 0.75W_{13}$$

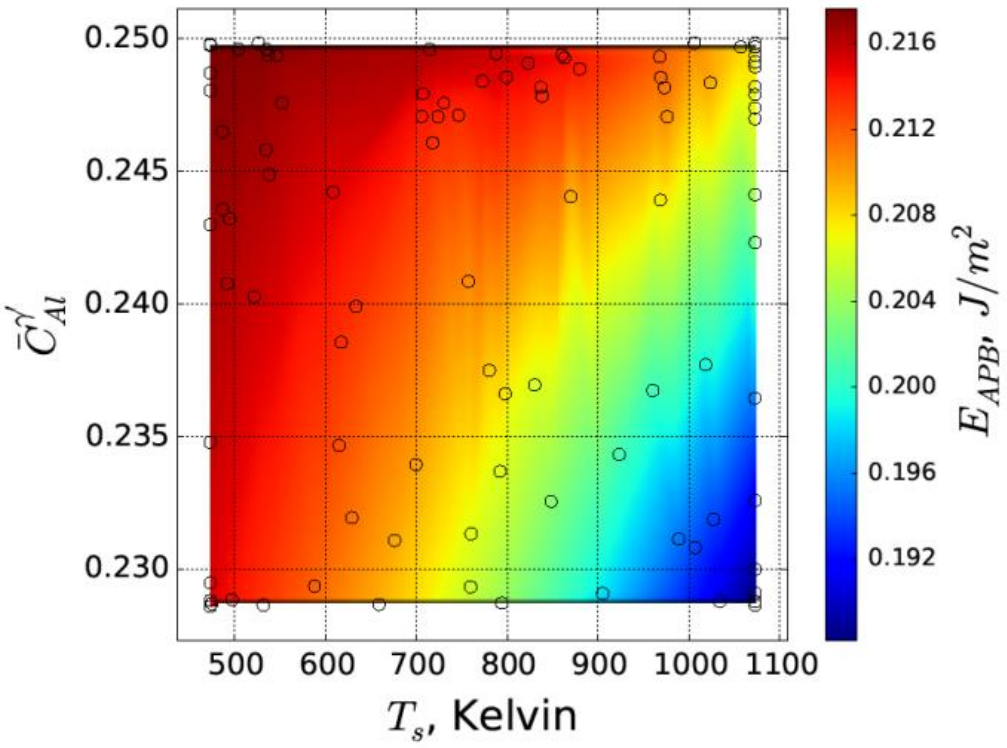
$$W_2 = \frac{\Delta H^{ORD}\left(1 - \bar{C}_s^{\gamma'}\right) - \bar{C}_s^{\gamma'}\Delta H^{FCC}}{12Rc^2\left(1 - \bar{C}_s^{\gamma'}\right)}$$

$$W_3 = 0.125W_{13}$$

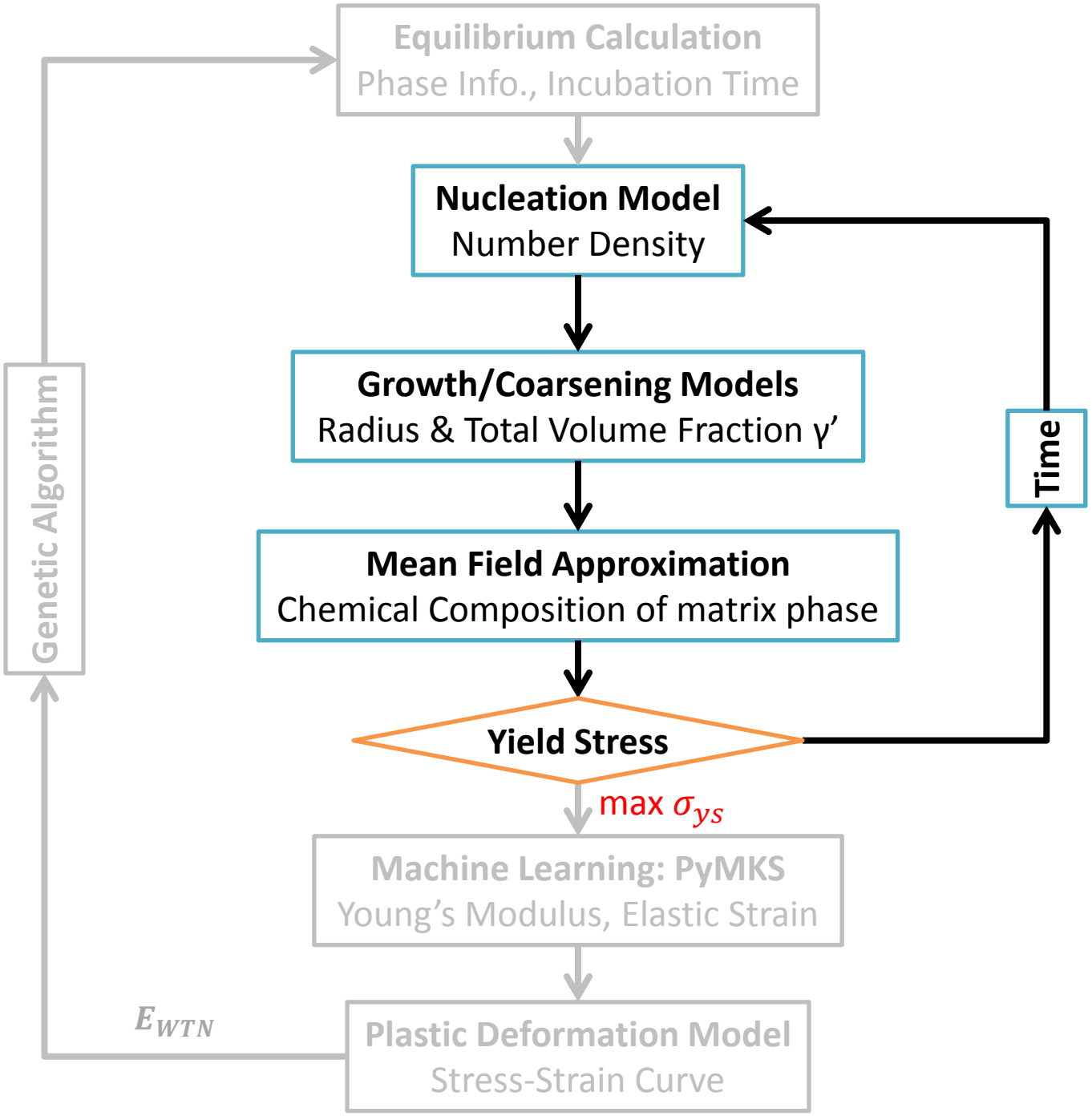
$$W_{13} = \frac{3\Delta H^{FCC} + \Delta H^{ORD}\dfrac{\left(1 - \bar{C}_s^{\gamma'}\right)}{\bar{C}_s^{\gamma'}}}{24Rc\left(1 - \bar{C}_s^{\gamma'}\right)}$$

$$= W_1 + 2W_3$$

Ni-Al



- Chemical composition $\bar{C}_{Al}^{\gamma'}$, $\bar{C}_{Cr}^{\gamma'}$ and lattice parameter of $a^{\gamma'}$ are calculated under equilibrium condition at T_p
- Chemical properties are obtained at T_s
- Chemical property of **Ni-Al-Cr** gives $E_{APB,[111]}$ =0.06-0.18 J/m^2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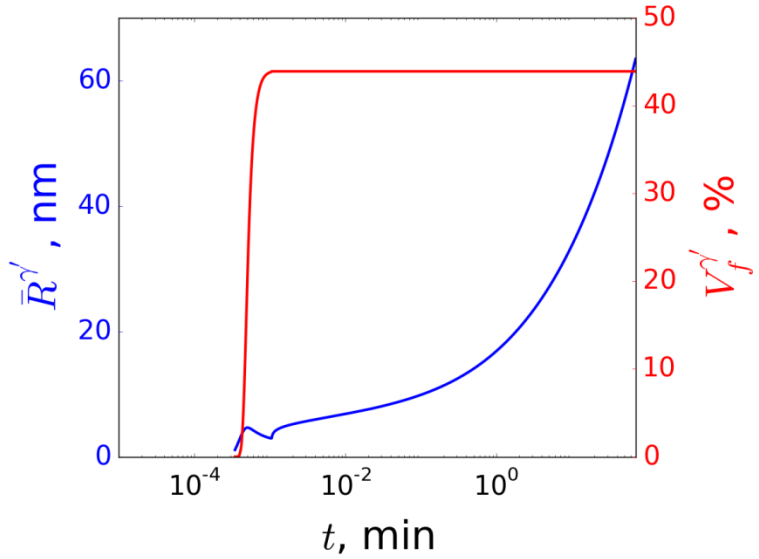
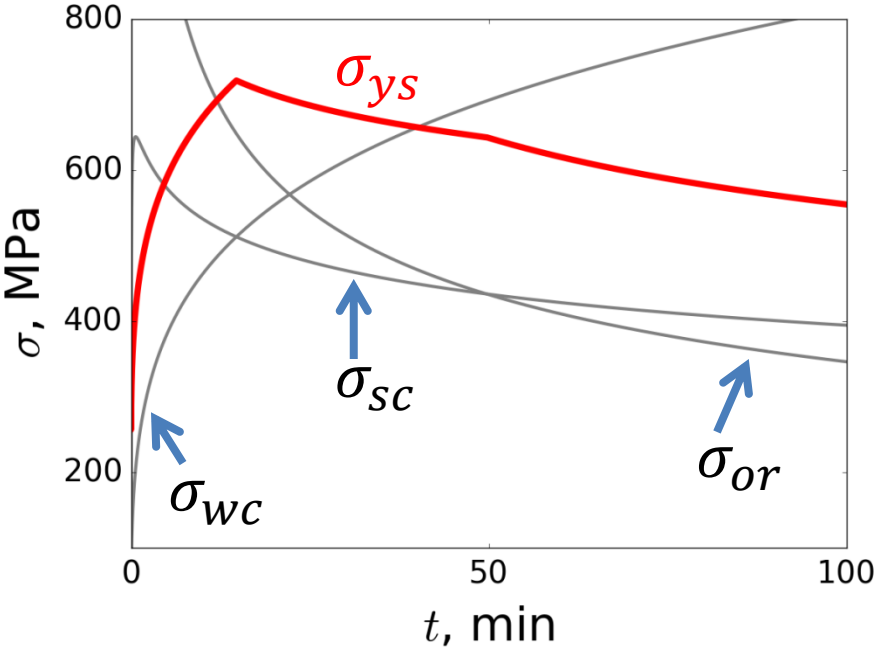
Process-Structure-Yield Stress

C_{Al}, %	13.62
C_{Cr}, %	17.46
T_p, Kelvin	1230
$V_{f,max}^{\gamma'}$, %	43.89
E_{int}, mJ/m²	25.51
E_{APB}, mJ/m²	118





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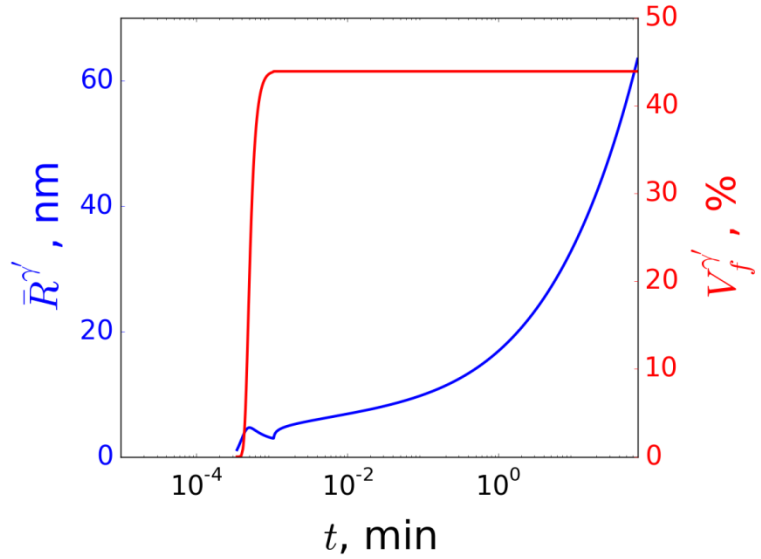
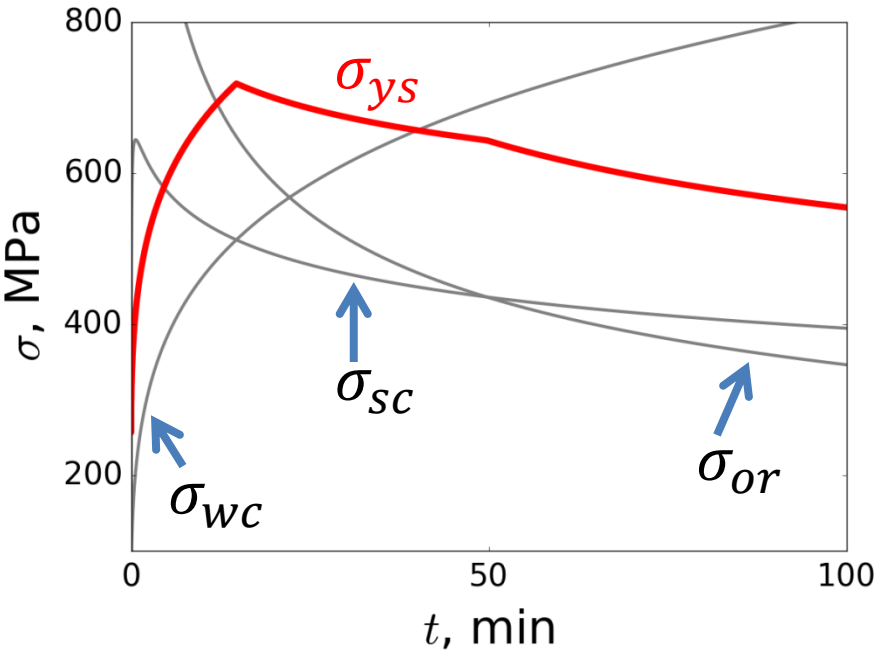
Average radius

$$\bar{R}^{\gamma'} = \frac{\sum N_c R_c^{\gamma'}}{\sum N_c}$$





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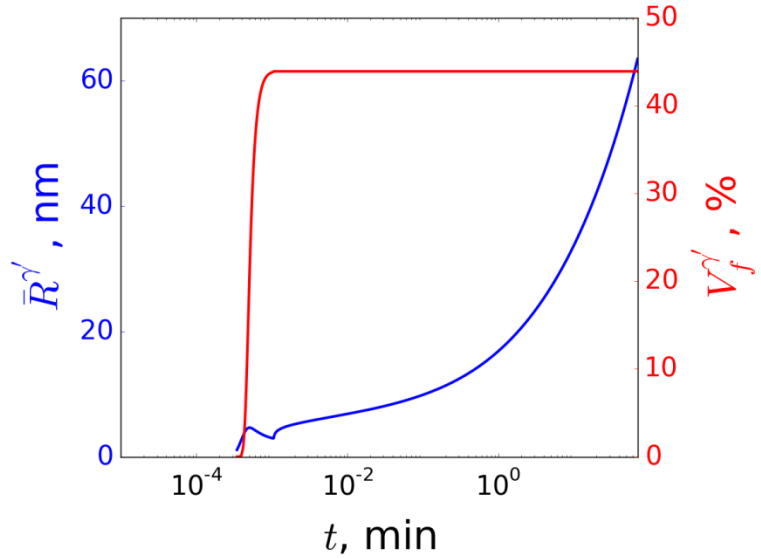
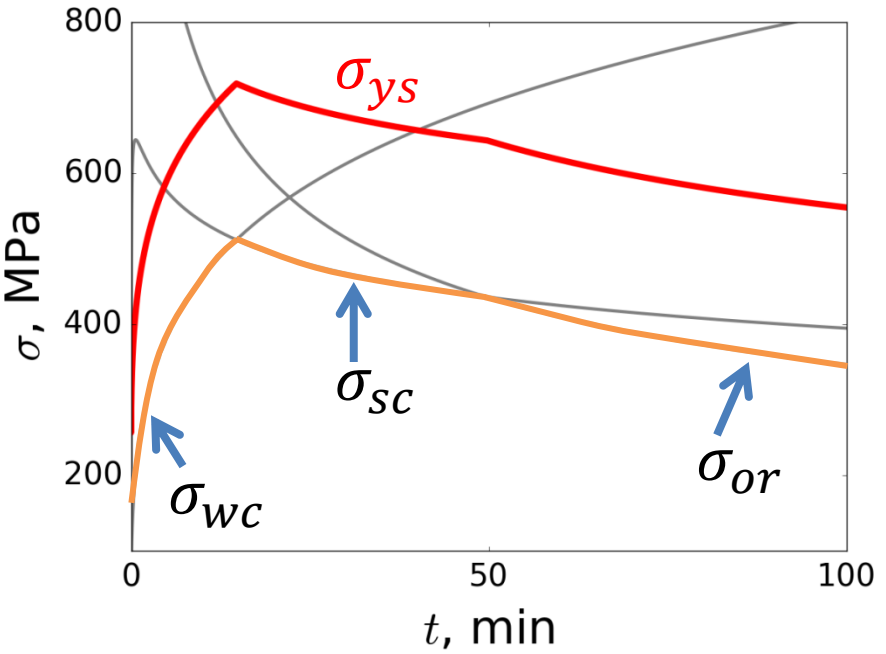
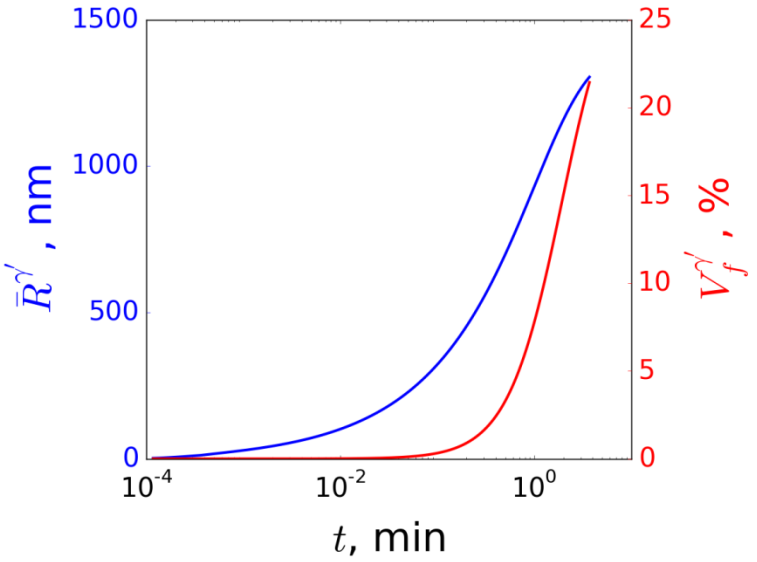
$$\bar{R}^{\gamma'} = \frac{\sum N_c R_c^{\gamma'}}{\sum N_c}$$

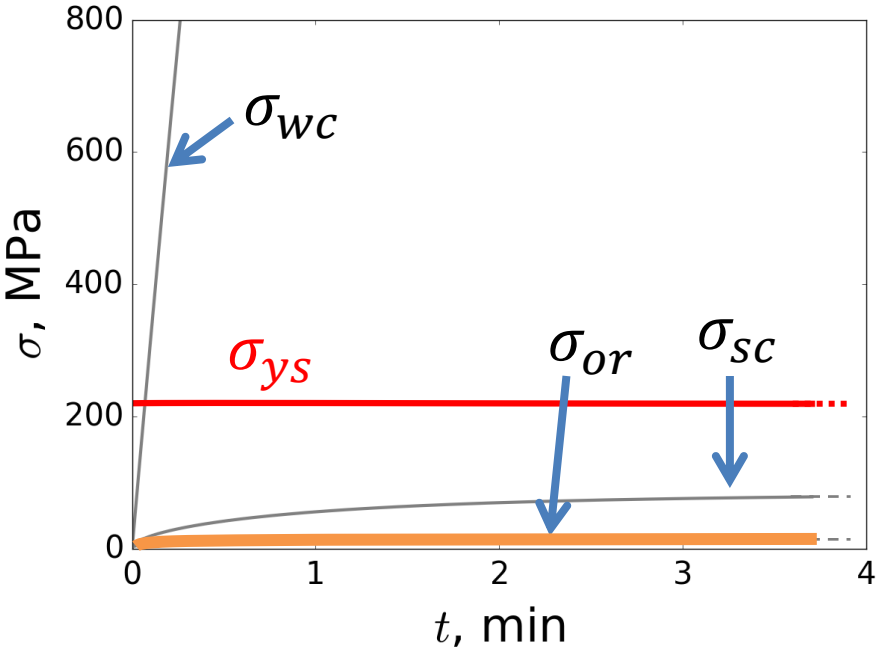


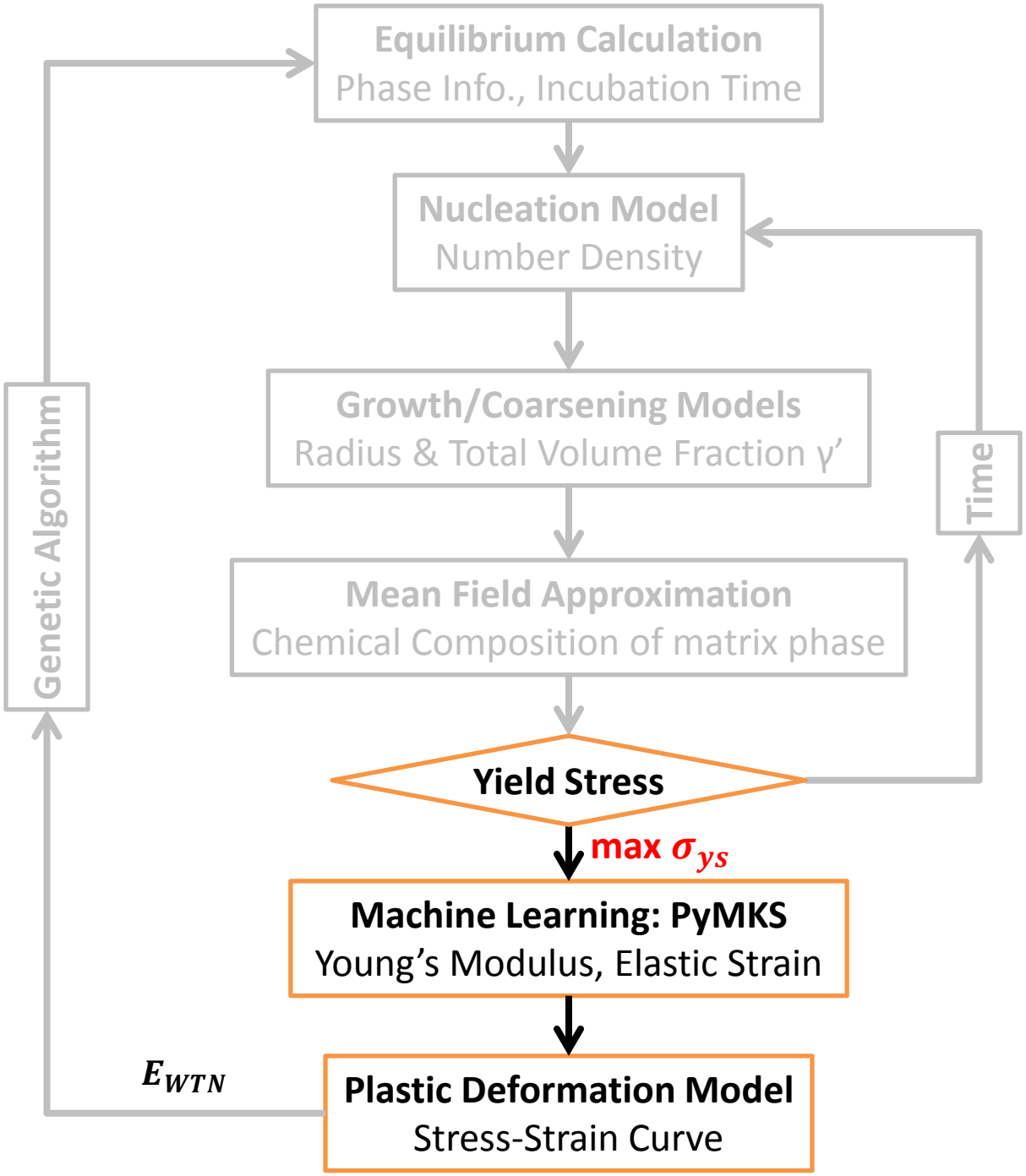


Process-Structure-Yield Stress

C_{Al}, %	14.05
C_{Cr}, %	10.16
T_p, Kelvin	1328
$V_{f,max}^{\gamma'}$, %	26.31
E_{int}, mJ/m²	27.47
E_{APB}, mJ/m²	157



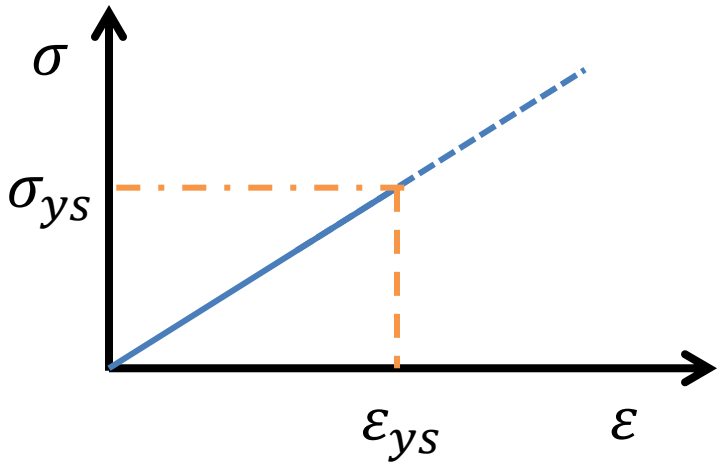


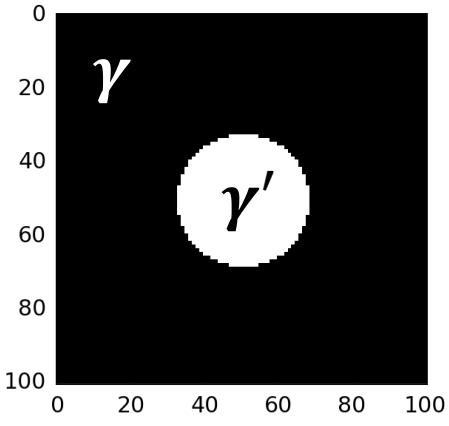

Equilibrium Calculation
Phase Info., Incubation Time
Nucleation Model
Number Density
Growth/Coarsening Models
Radius & Total Volume Fraction γ'
Mean Field Approximation
Chemical Composition of matrix phase
Yield Stress
max σ_{ys}
Machine Learning: PyMKS
Young's Modulus, Elastic Strain
Plastic Deformation Model
Stress-Strain Curve
E_{WTN}
Genetic Algorithm
Time

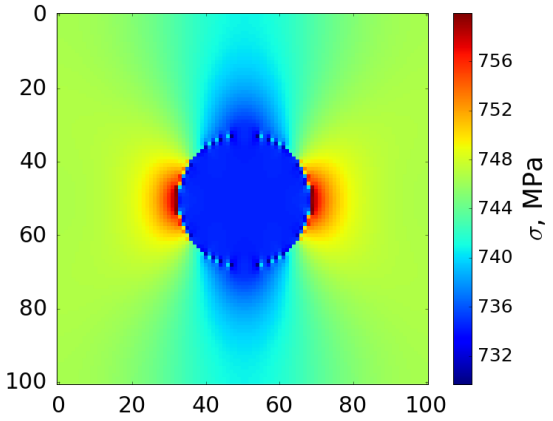
Machine Learning Tech for Elastic Deformation – PyMKS

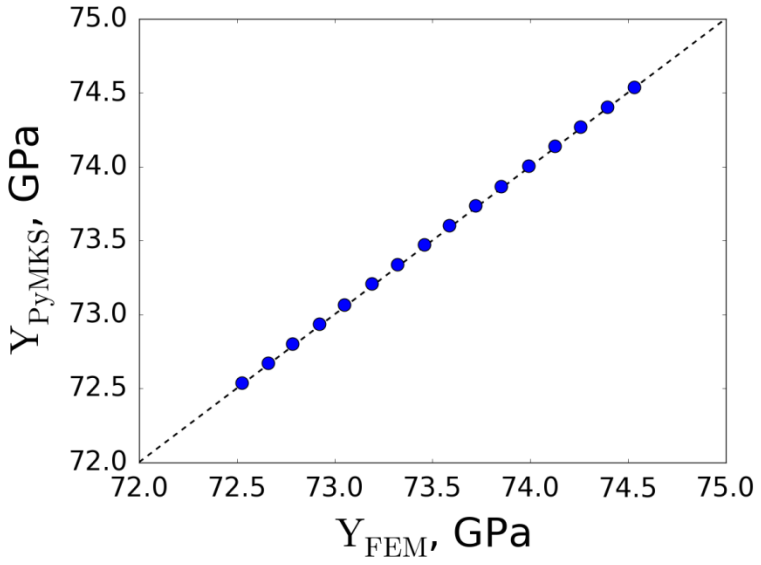
Fast et al., 2011
Kalidindi, 2012

- Statistical/machine learning tool correlating microstructure with properties by linear function
- By employing machine learning technique, PyMKS can reproduce the FEM calculations in a more efficient way
- For the microstructure with high volume fraction of γ', the representative volume element is created for PyMKS calculation









Plastic Deformation Model

Mecking et al., 1986
Huang et al., 2007, 2008

The evolution of the dislocation density (ρ) is calculated as increasing strain based on non-equilibrium thermodynamics and Kocks-Mecking model using shear modulus (μ), burger's vector (b), mean free path of dislocation (l), vibration frequency (ν_0), energy barrier of dislocation annihilation (ΔG_ρ) and model constant (C, α)

$$\rho_{in,\varepsilon+\Delta\varepsilon} = \rho_{in,\varepsilon} + \frac{(\mu b^2 + \tau b l)\frac{\nu_0}{\dot{\varepsilon}} exp\left(-\frac{\Delta G_\rho}{kT}\right)\rho_{in,\varepsilon} - \tau_\rho}{\frac{1}{2}C\alpha\mu b^2 - (\mu b^2 + \tau b l)}\Delta\varepsilon$$

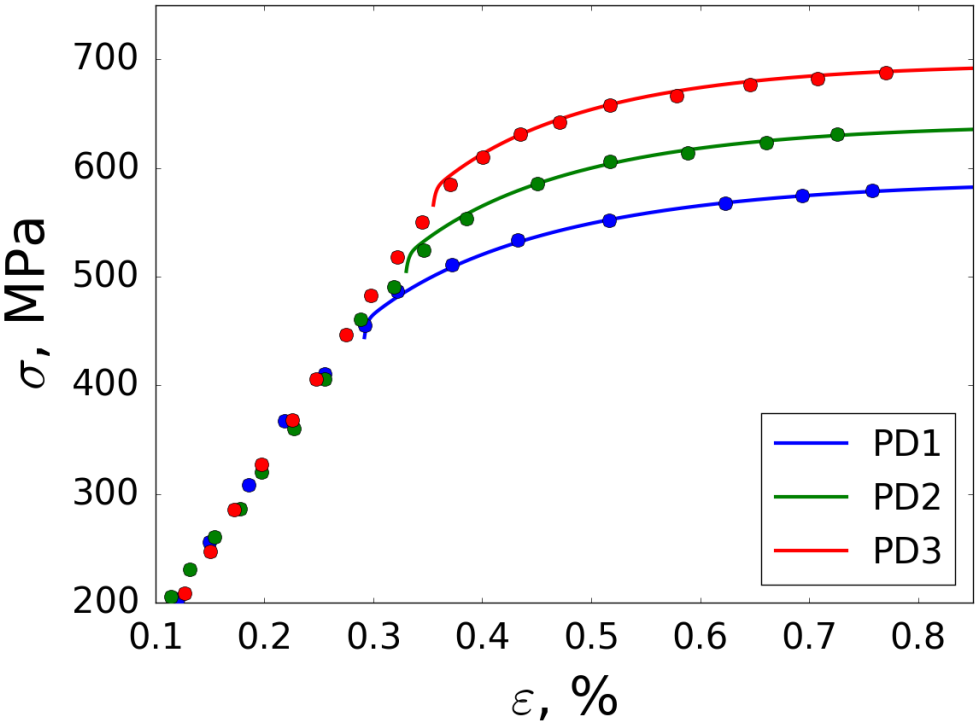
$\Delta\varepsilon$

$$M\tau = \sigma_0 + \sigma_{SS} + \sigma_{H-P} + \sqrt{\sigma_\rho^2 + \sigma_p^2}$$

Plastic Deformation Model

Le Baillif et al., 2014

	$V_f^{\gamma'}$	σ_{ys}, MPa	ε_{ys}, %
PD1	0.323	450	0.29
PD2	0.296	560	0.33
PD3	0.278	570	0.36



- $T_s = 1123K$
- PD1 is used for calibration
- $\Delta G_\rho = 3.08$ eV and $C = -180$ provide the best agreement to PD1

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Le Baillif et al., 2014

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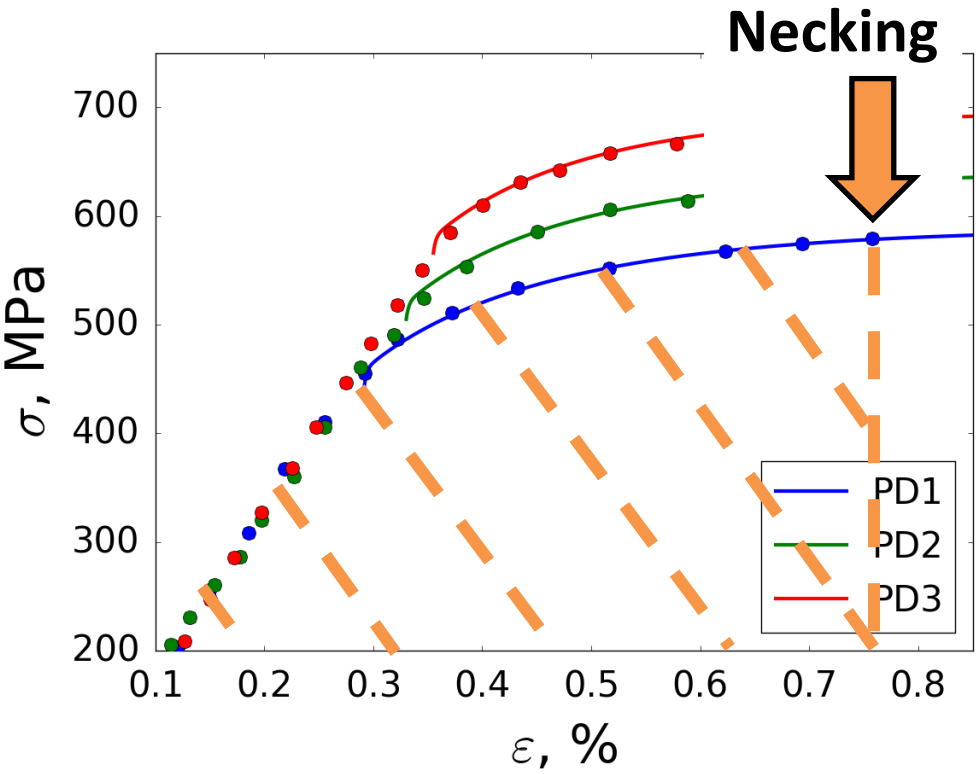

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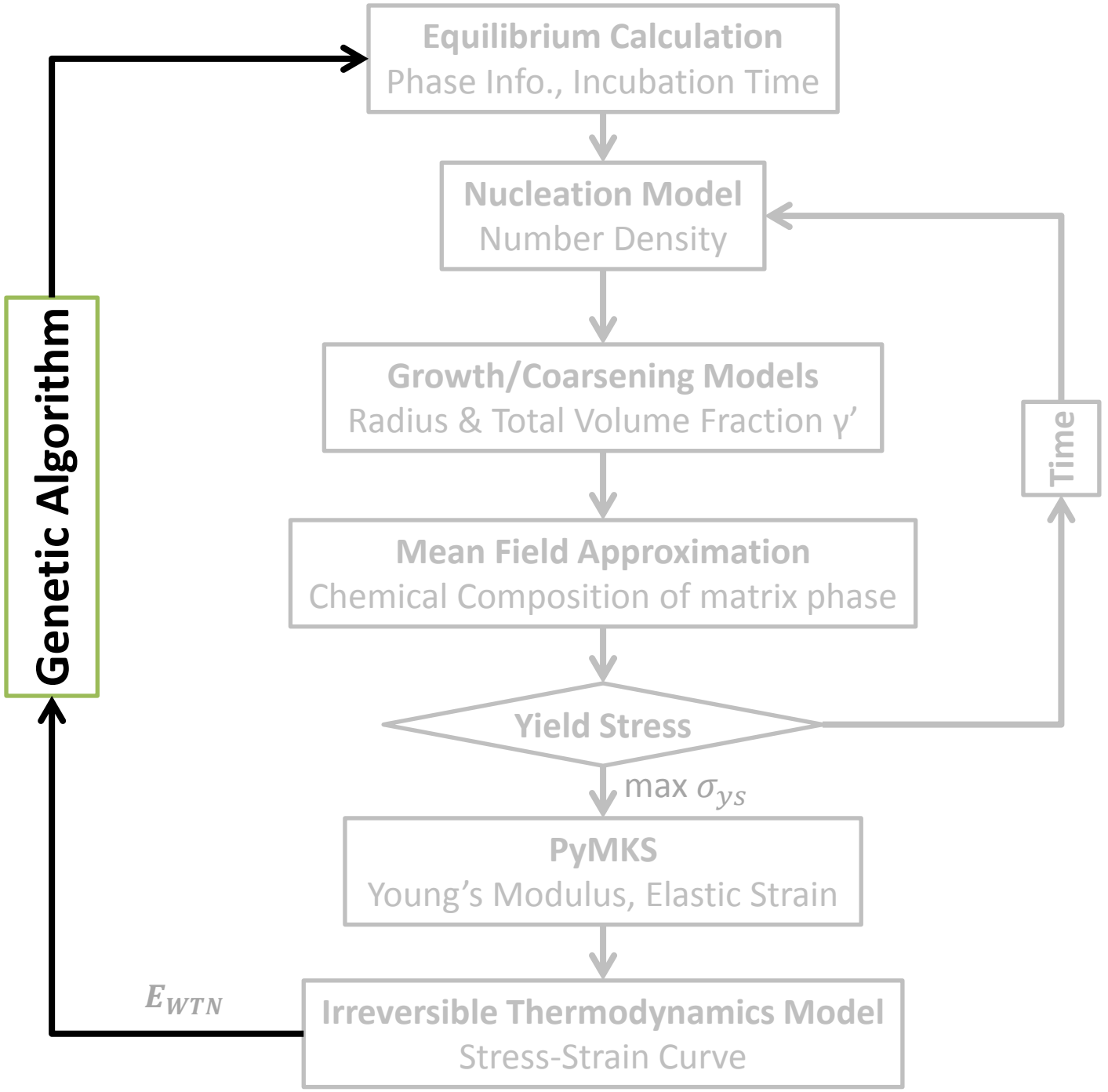
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E_{WTN}
Genetic Algorithm
Time

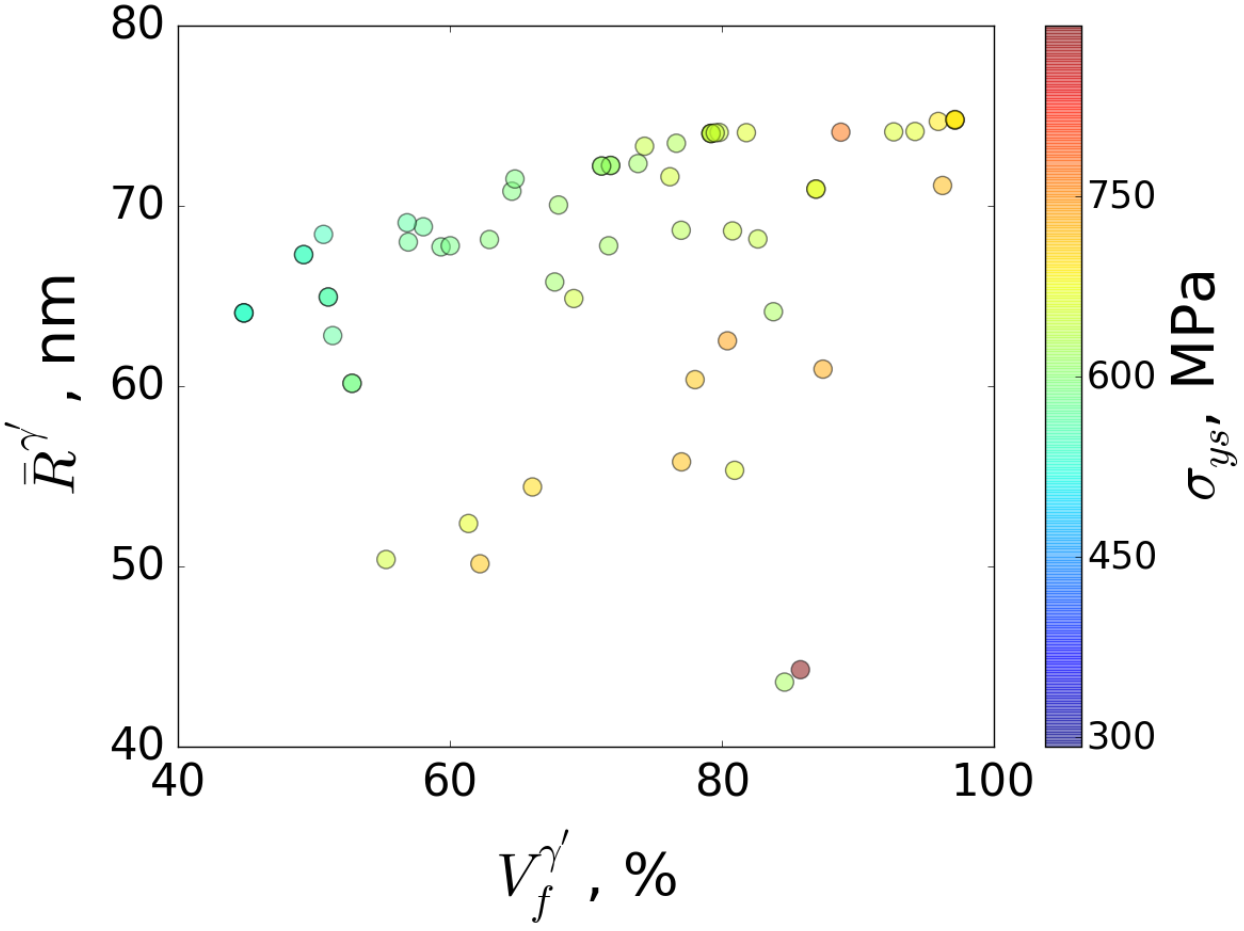
Optimization

Input conditions

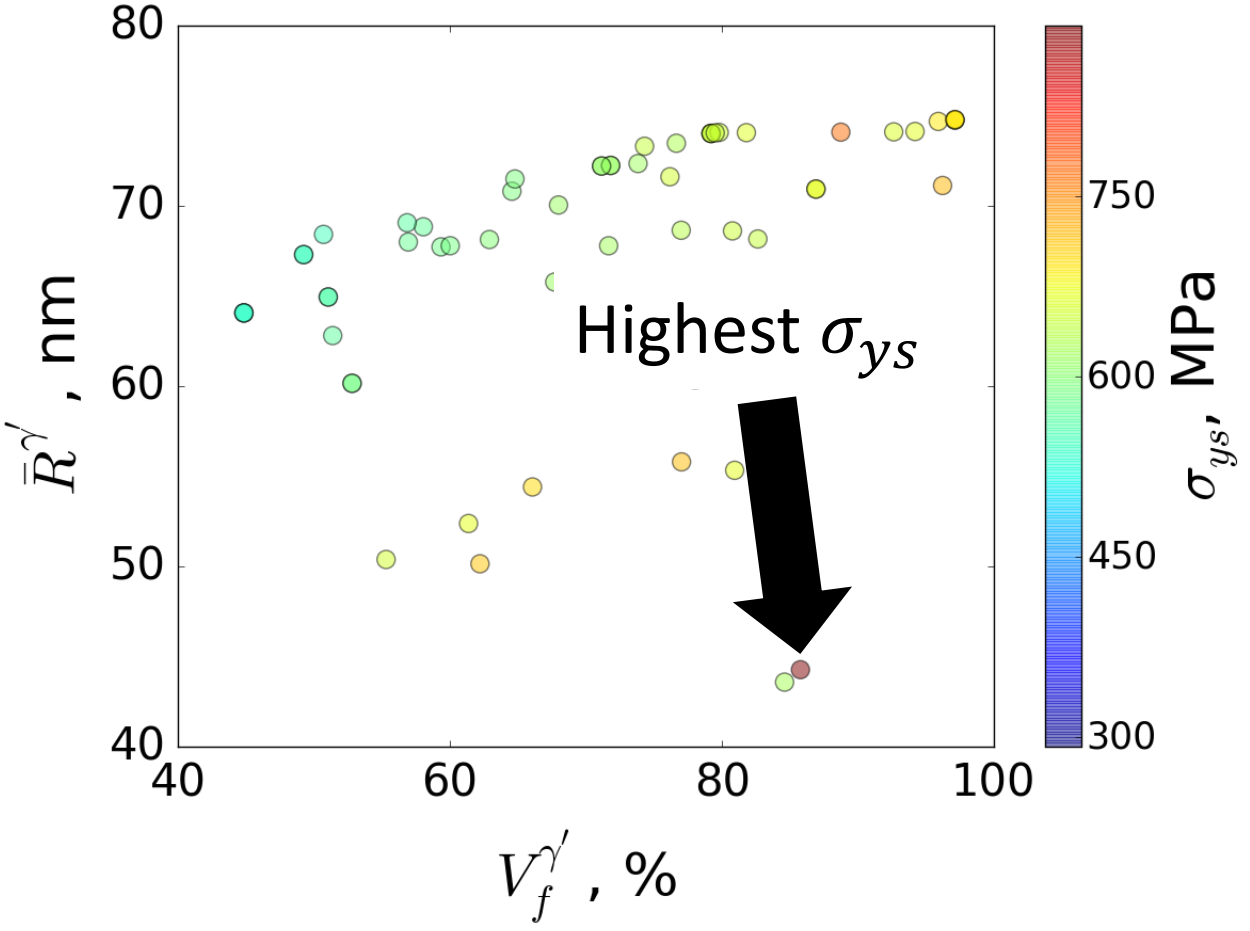
	C_{Al}, %	C_{Cr}, %	T_p, K
Min	10	10	1123
Max	25	20	1473

- Objective: high **work to necking (E_{WTN})** at $T_s = 1123K$
- Pass the calculations while $\bar{V}_f^{\gamma'} < 0.4$
- 6 bits of memory is utilized for 1 variable
- 6 samples are selected in 1 generation and 10 generations are calculated

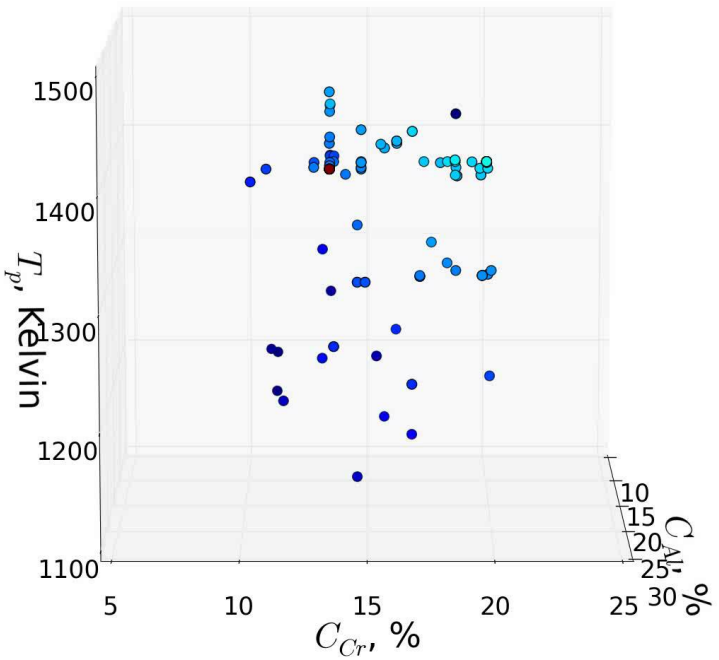
Optimization

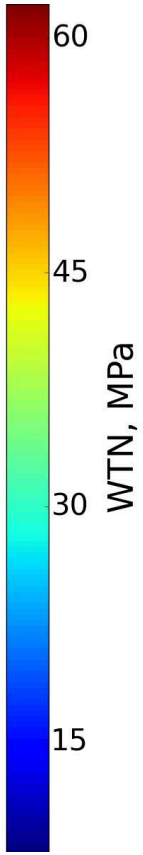


Optimization

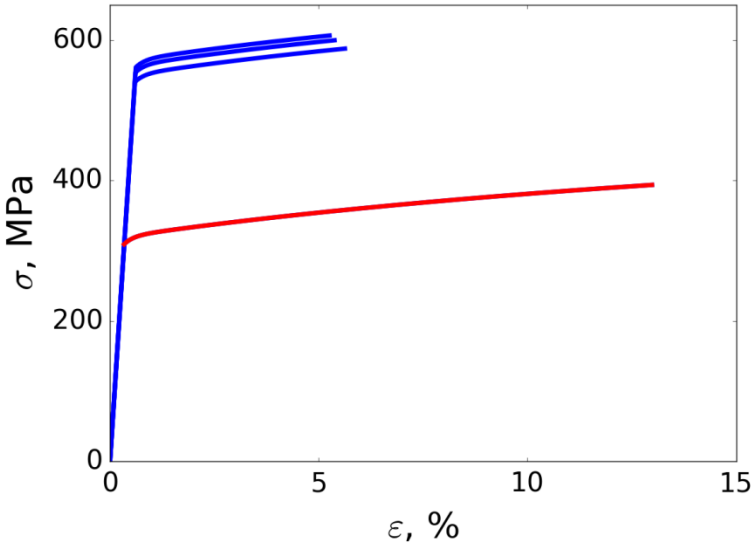


Optimization - WTN





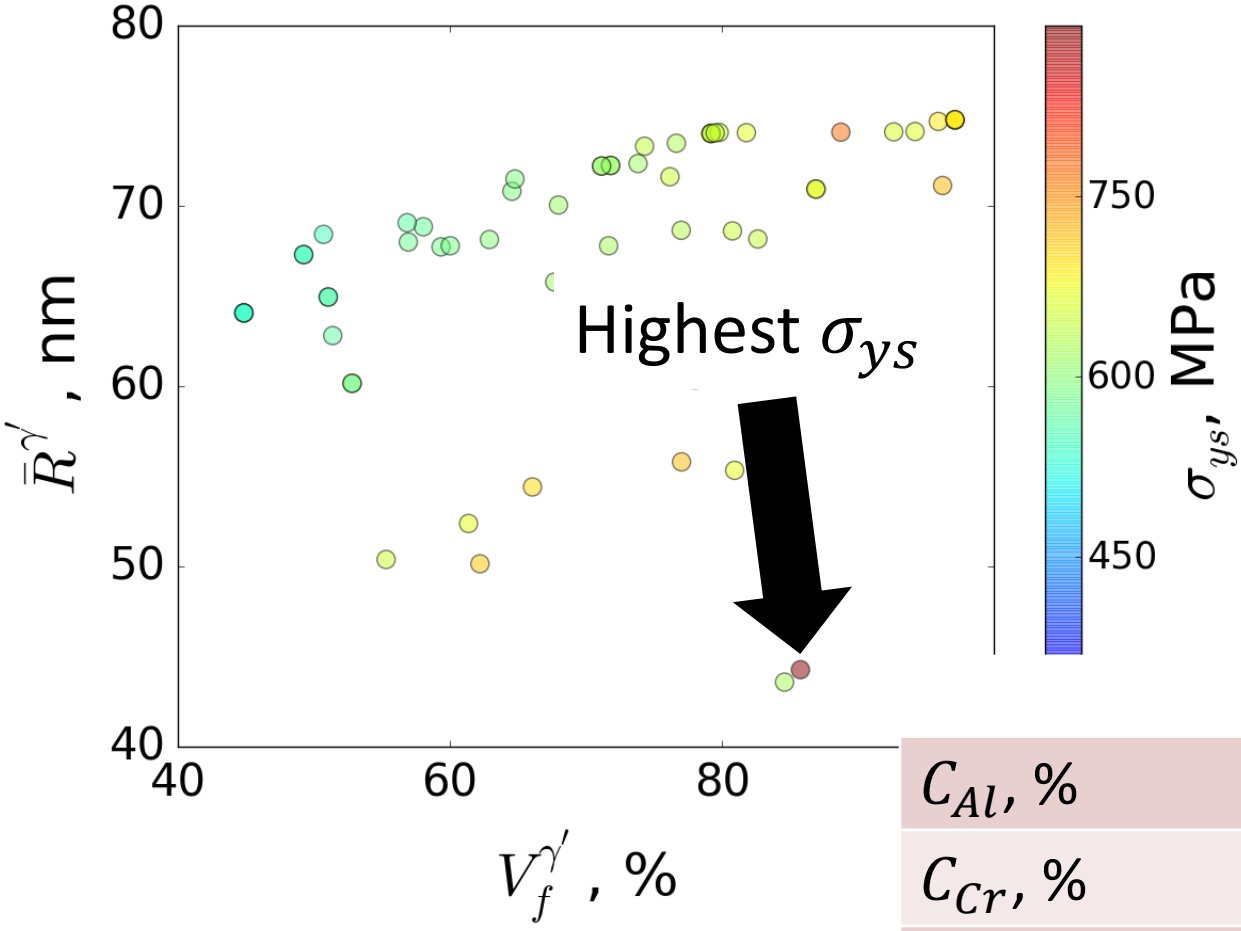
C_{Al}, %	0.231
C_{Cr}, %	0.195
T_p, Kelvin	1450
σ_{UTS}, MPa	394
ε_{UTS}, %	12.98



Summary

- The optimization of Ni-Al-Cr ternary system is demonstrated.
- With proper E_{INT} and N_0, nucleation-growth-coarsening models successfully approach γ' precipitation in binary and ternary system.
- The yield stress and young's modulus are calculated by empirical formulas and PyMKS package, respectively.
- The IRT model is implemented to simulating the plastic deformation.
- To optimize the chemical composition, Genetic Algorithm is used as the close loop of process-structure-properties.

Optimization



C_{Al}, %	0.174
C_{Cr}, %	0.110
T_p, Kelvin	1250
σ_{ys}, MPa	891