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Predicting Matrix Phase Composition and Properties Using CALPHAD-Guided Thermokinetic Simulations with MatCalc

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Simulation Approach

Investigate matrix phase composition and properties across wide variations of alloy chemistries.

- **CALPHAD**-based simulation approach using the **MatCalc** toolbox.
- Systematic variation of chemical composition to explore alloying effects.

Focus Areas:

- Phase stability
- Transformation kinetics
- Mechanical properties

Key Enablers:

- accurate **thermodynamic databases**
- Robust **kinetic modeling**

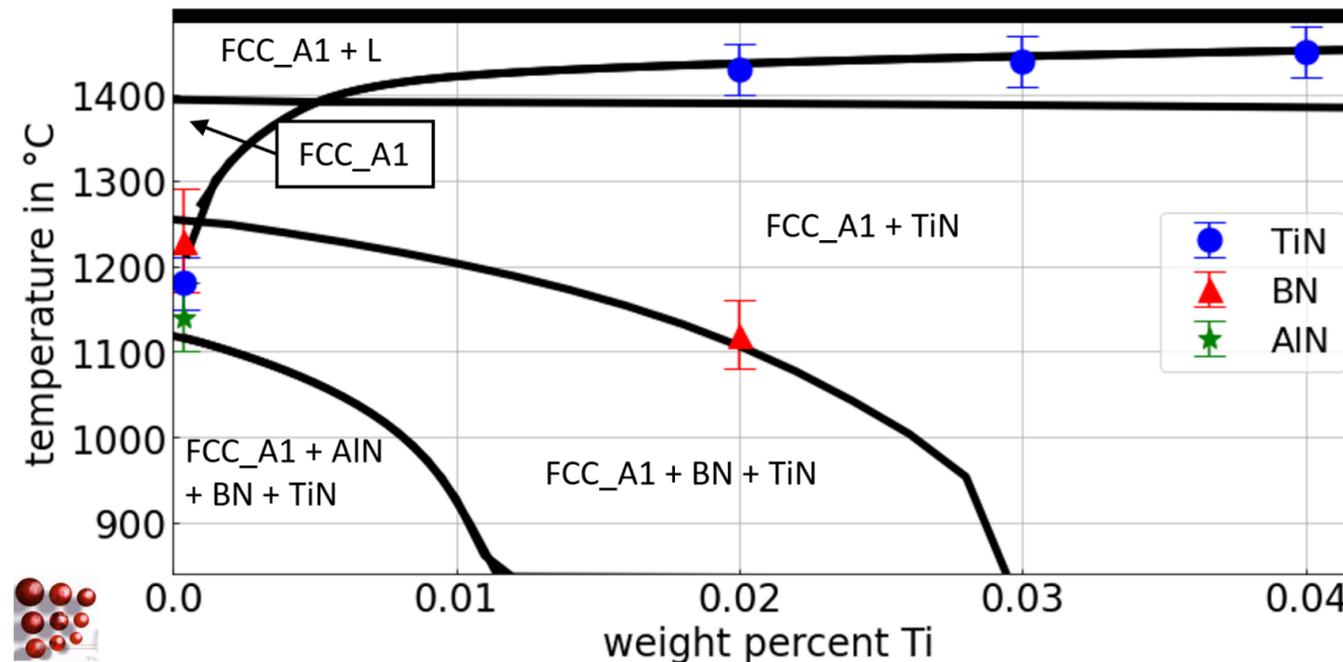
Benefits:

- **Reliable predictions** under realistic processing conditions
- Significant reduction in development time
- Minimization of experimental trials

Innovation Potential:

- **Real-time** adaptation of process parameters during production
- Enhanced **efficiency and responsiveness** in manufacturing workflows

Pseudobinary phase diagram with varying Ti-fraction [1]
(0.5 wt.-% C, 79 wt.- ppm N, 0.03 wt.-% Al, and 36 wt.-ppm B)



Boron in Steel

Increasing the through hardenability ~ 30wt.-ppm

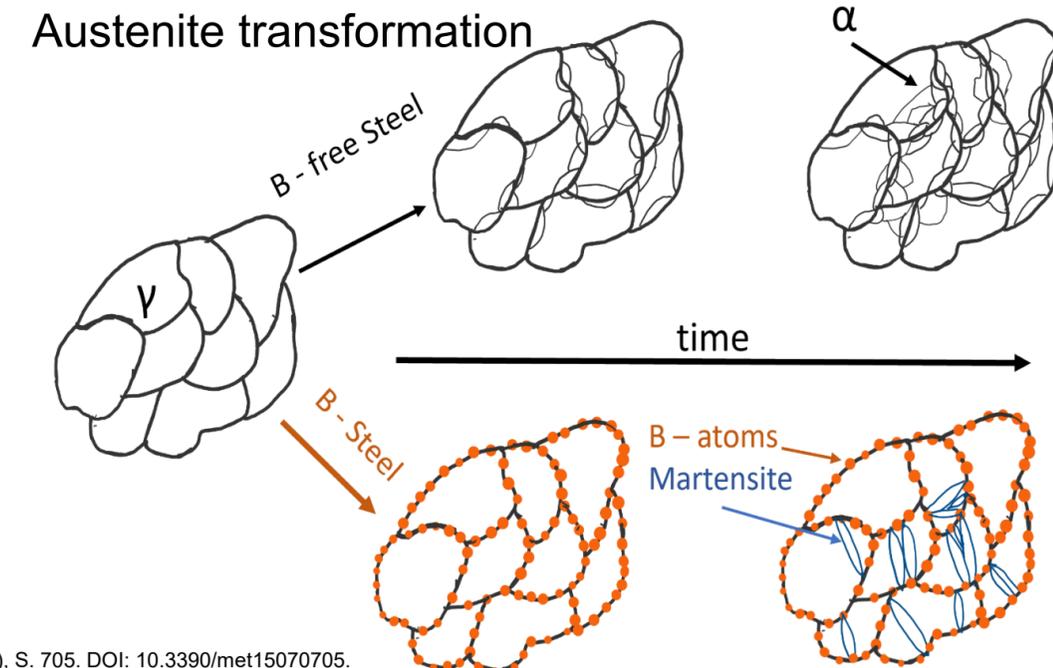
- Boron at γ -grain boundaries
- restricts nucleation of ferrite
- Tends to form BN

in ferritic/pearlitic structures in the cementite of pearlite

in austenite:

- in former pearlite regions (after short annealing)
- at austenite grain boundaries (after long annealing)

Rule of thumb: > 10 wt.ppm in SS for good B performance





Modeling approach

Precipitation simulation in MatCalc [1]

Thermodynamics/mobility: calphad-type database

$$G = \sum N^\alpha G_m^\alpha(T, P, x_i)$$

Nucleation: classical nucleation theory (CNT)

$$J = N_0 Z \beta e^{\frac{G^*}{kT}} e^{-\frac{\tau}{t}} \quad G^* = \frac{16}{3} \pi \frac{\gamma^3}{\left(\Delta G_0 - \frac{aE\varepsilon^2}{(1-\nu)}\right)^2}$$

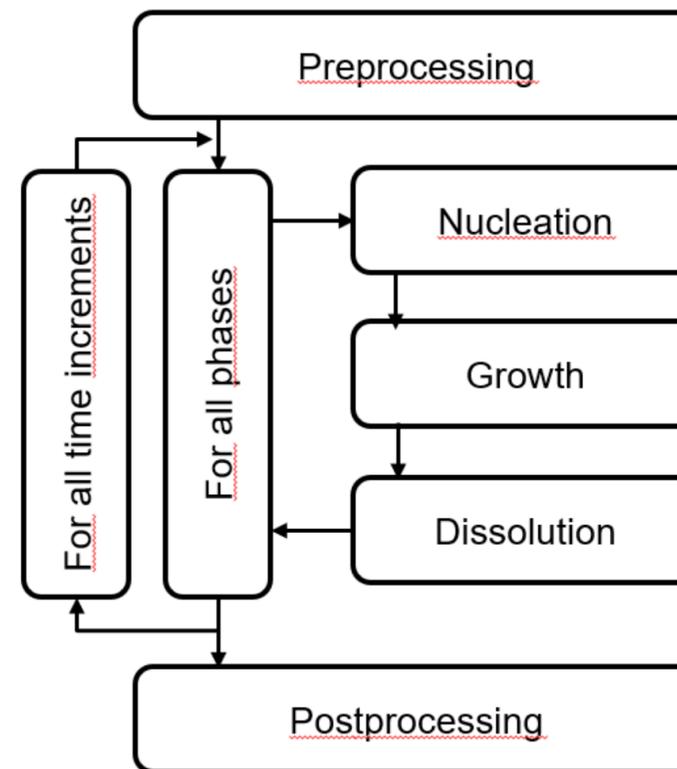
Kinetic model: Numerical Kampmann-Wagner

Interfacial energies: generalized nearest-neighbor broken-bond [3]

$$G = \sum_{i=1}^n N_{0,i} \mu_{0,i} + \sum_{k=1}^m \frac{4\pi\rho_k^3}{3} \left(\lambda_k + \sum_{i=1}^n c_{k,i} \mu_{k,i} \right) + \sum_{k=1}^m 4\pi\rho_k^2 \gamma_k$$

Evolution equations (TEP [2])

Matcalc Workflow



Grain growth model

Change in grain diameter \dot{D}

$$\dot{D} = M_{\text{eff}} \cdot \Delta P = M_{\text{eff}} \cdot (P_D - P_Z) \quad [4]$$

driving pressure

$$P_D = k_d \cdot \frac{\gamma_D}{D}$$

retarding force

$$P_Z = k_r \cdot \frac{\gamma_D f_v}{r}$$

Mobility pinned interface M_p

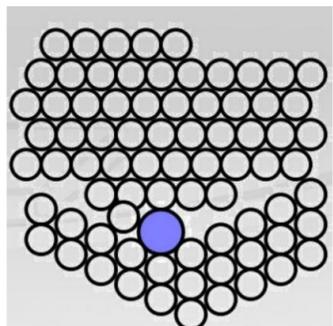
$$M_p = \eta_p \eta_f \frac{\omega D_{\text{CB,Fe}} V_M}{b^2 RT}$$

Mobility solute Drag effect M_{SD} (Cahn [5,6])

$$M_{\text{SD}} = \frac{1}{c_{\text{GB}} \frac{\omega(RT)^2}{E_B D_{\text{CB}} V_M} \left[\sinh\left(\frac{E_B}{RT}\right) - \frac{E_B}{RT} \right]}$$

effective mobility M_{eff}

$$\frac{1}{M_{\text{eff}}} = \frac{1}{M_{\text{int}}} + \frac{1}{M_p} + \frac{1}{M_{\text{SD}}}$$



[1] Kozeschnik, Ernst (2022): Mean-Field Microstructure Kinetics Modeling (In: Francisca G. Caballero (ed.), Encyclopedia of Materials: Metals and Alloys. vol. 4.), S. 521–526

[2] Svoboda, J.; Fischer, F. D.; Fratzl, P.; Kozeschnik, E. (2004): Modelling of kinetics in multi-component multi-phase systems with spherical precipitates. In: Materials Science and Engineering:A 385 (1-2), S. 166–174.

[3] Sonderegger, B.; Kozeschnik, E. (2010): Interfacial Energy of Diffuse Phase Boundaries in the Generalized Broken-Bond Approach. In: Metallurgical and Materials Transactions A 41 (12), S. 3262–3269.

[4] J. E. Burke, D. Turnbull, Prog. Met. Phys. 1952, 3, 220.

[5] J. W. Cahn, Acta Metall. 1962, 10, 789.

[6] H. Buken, E. Kozeschnik, Metall. Mater. Trans. A 2017, 48, 2812.



Thermokinetic Simulation Results

B in solid solution – Grain size evolution

Simulation setup

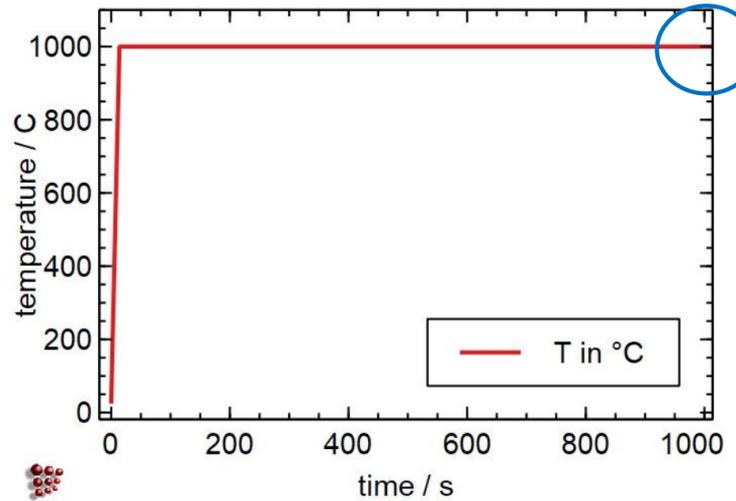
Alloying system microalloyed steel

C	Mn	Cr	Si	S	Al	B	N	Ti
0.2	0.9	0.25	0.07	0.01	var	var	var	var

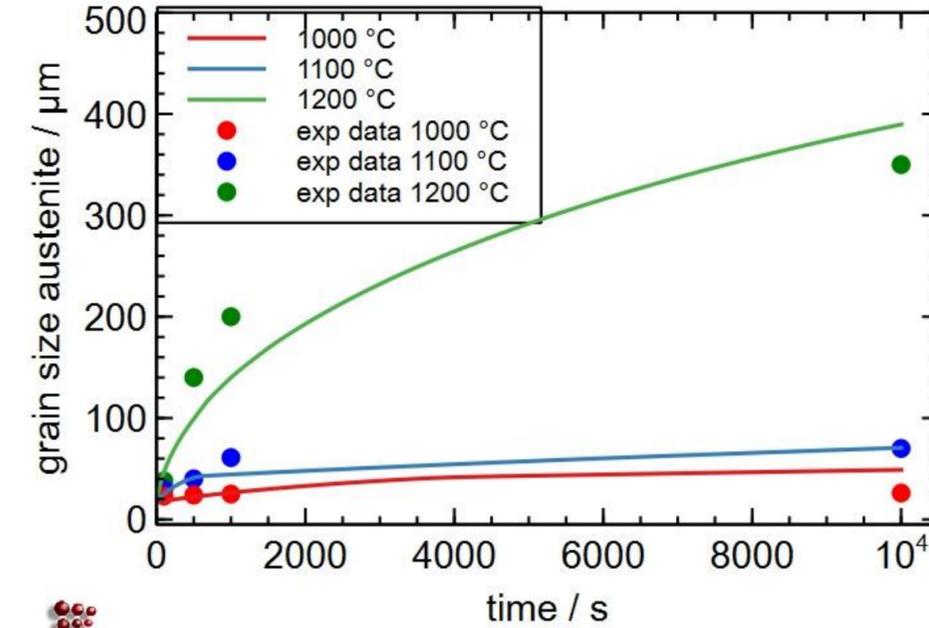
Variation of elements in microalloyed steel:

- **Al** (0.010 – 0.070 wt. % (50 ppm))
- **B** (0.002 – 0.005 wt. % (2 ppm))
- **N** (0.005 – 0.02 wt. % (10 ppm))
- **Ti** (0.018 – 0.062 wt. % (20 ppm))

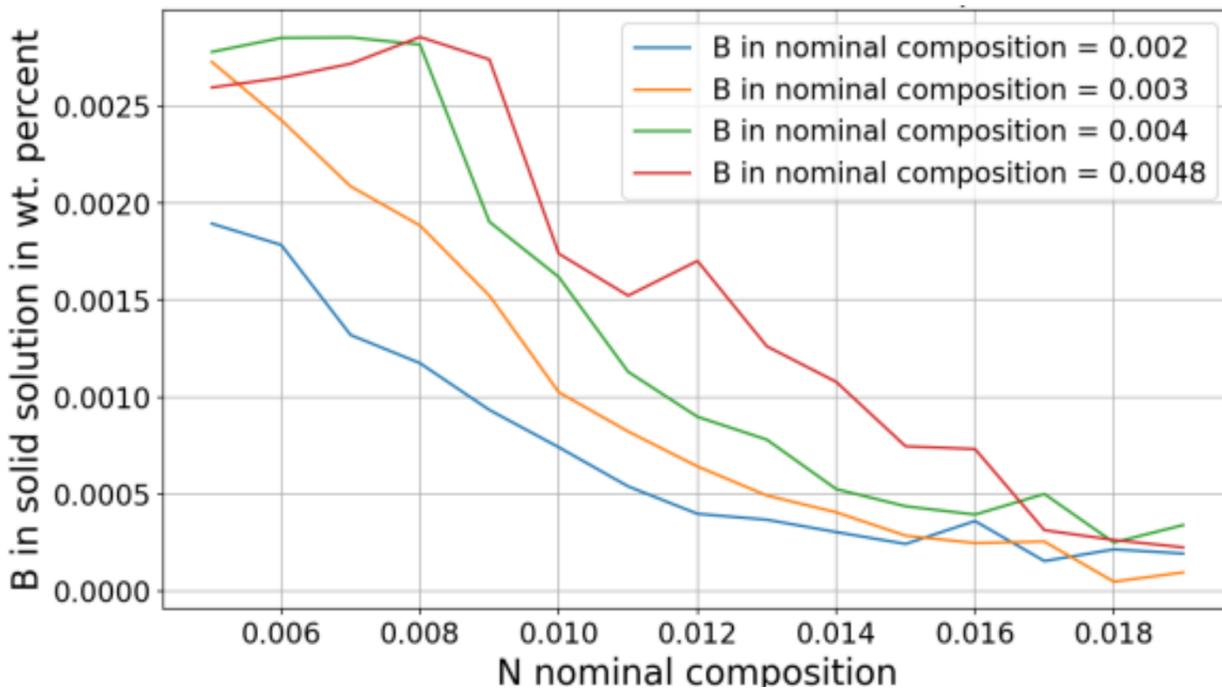
Austenitization heat treatment
Matrix composition prior to quenching
relevant for investigation



Evolution grain size

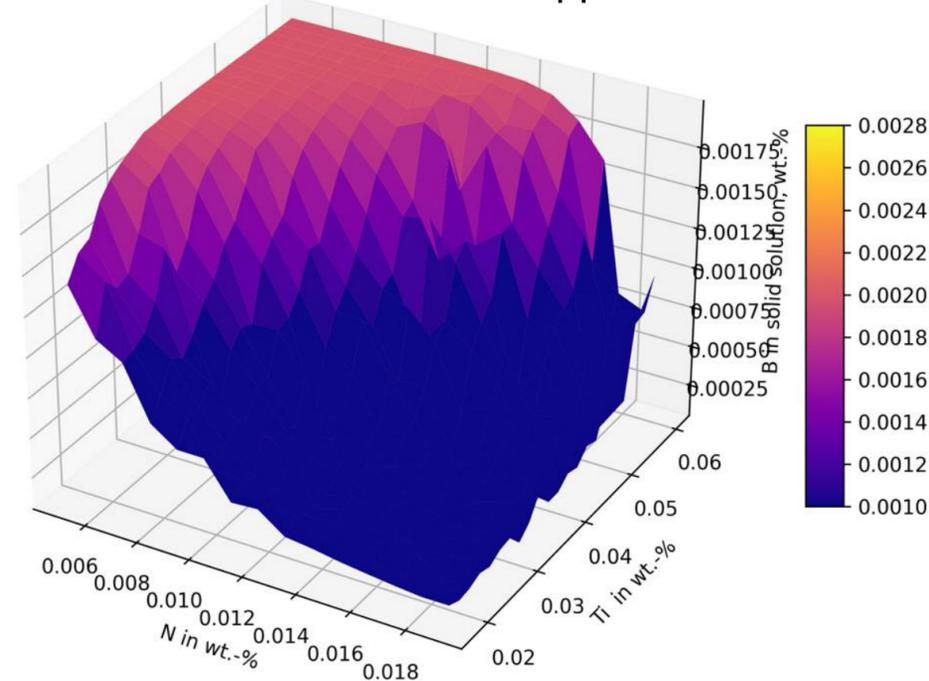


Fraction of **Boron** in solid solution in relation to **N** fraction
Al=0.04, Ti=0.03



Fraction of **Boron** in solid solution in the matrix

Nominal B-fraction 20. wt-ppm



Nominal B-fraction 40 wt.-ppm

