A Combinatorial Approach to the Study of the Solute Drag Effect of Nb on Ferrite Grain Boundary Motion

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Nb Solute Effects on Grain Boundary Motion in α

Cahn (1962), Hillert (1969, 1976) – Models for solute effects are available

Use of the models requires knowledge of parameters – E_b, D^{trans}, M_{int}; (X,T)

Experimentally we must use UHP materials containing extremely low C levels to avoid NbC precipitation (which will complicate interpretation and quantification)

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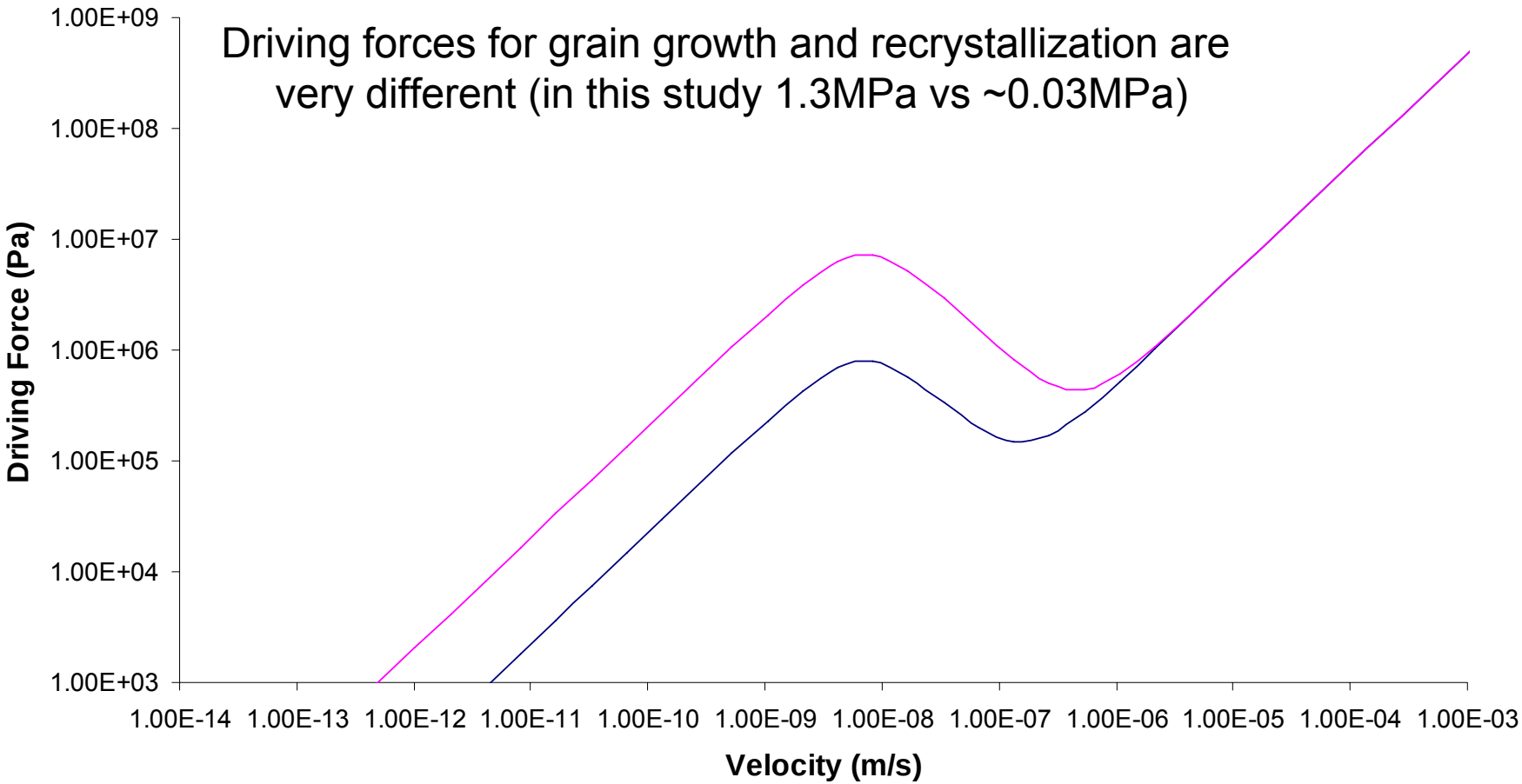
We have used a 'combinatorial approach' to the question of solute Nb effects on recrystallization and grain growth in UHP α-Fe

Experimentally examine the behavior under simultaneous gradients in Nb and T

What Consititutes High and Low Driving Forces?

We also obtain some idea of SD branch selection



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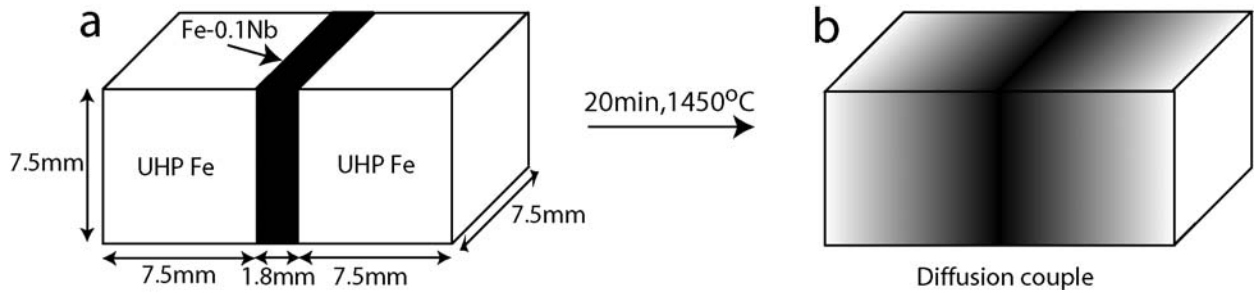
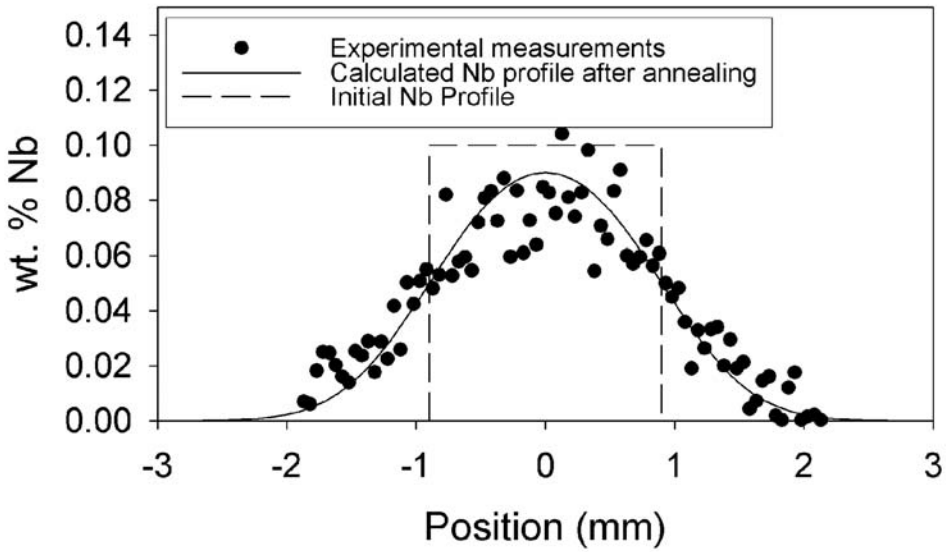
Sample Preparation





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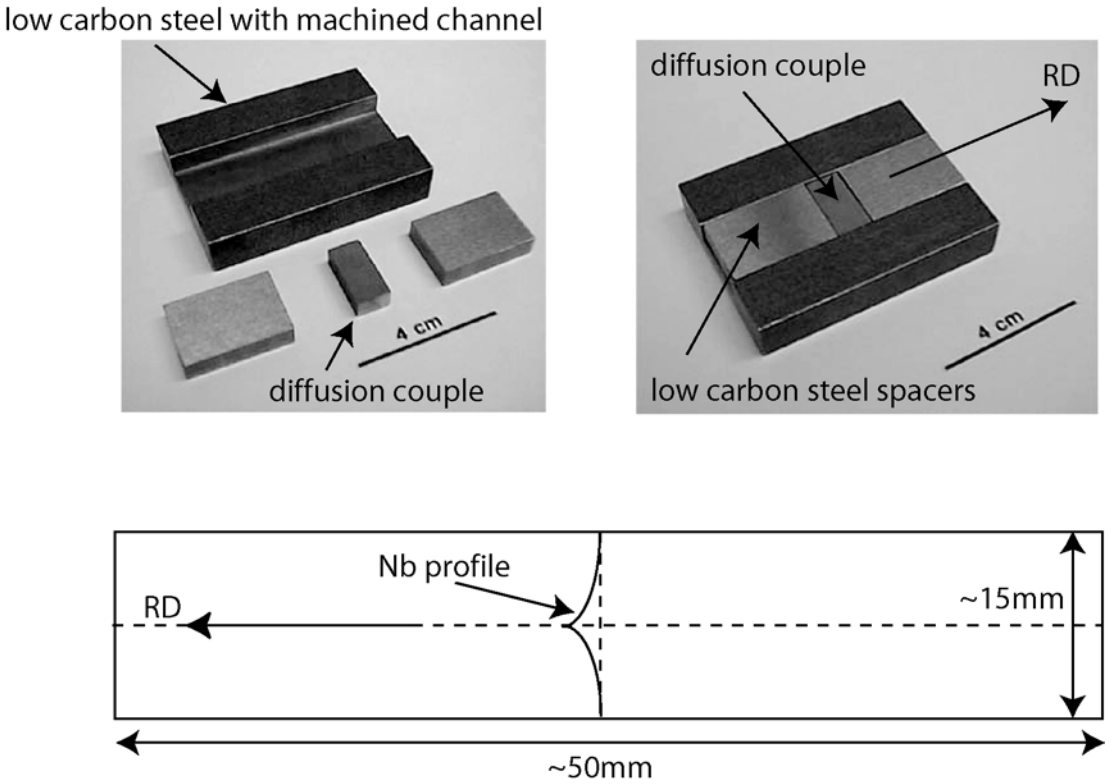
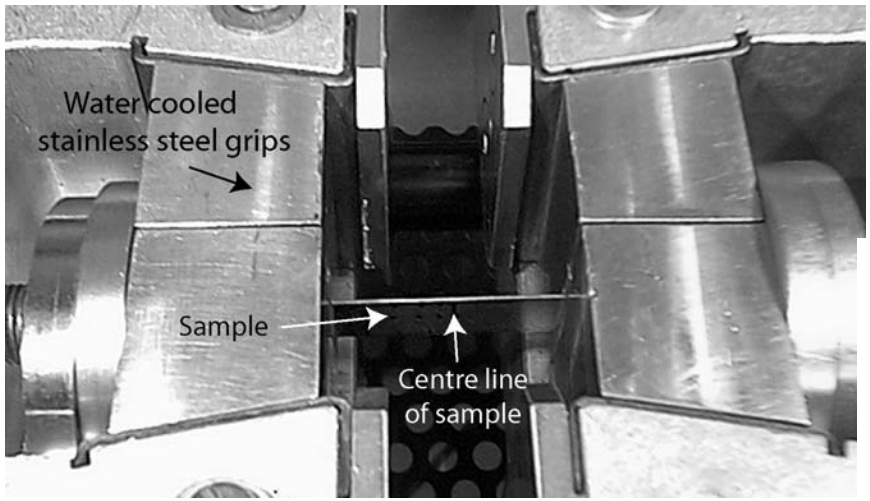
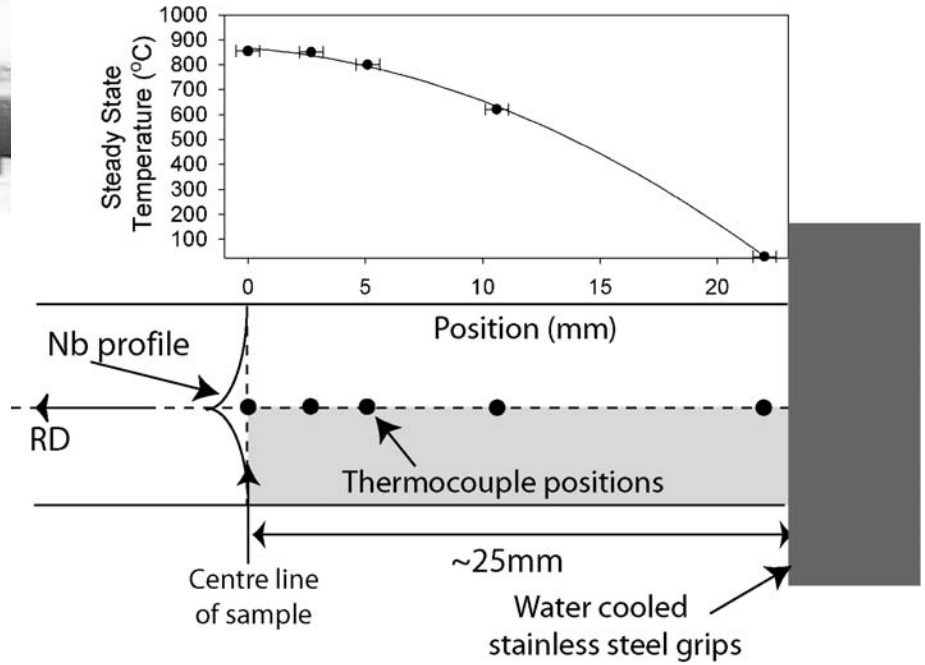


Nb Solute Effects on Grain Boundary Motion in α

Experimental Set-up



Gleeble Thermo-mechanical Simulator



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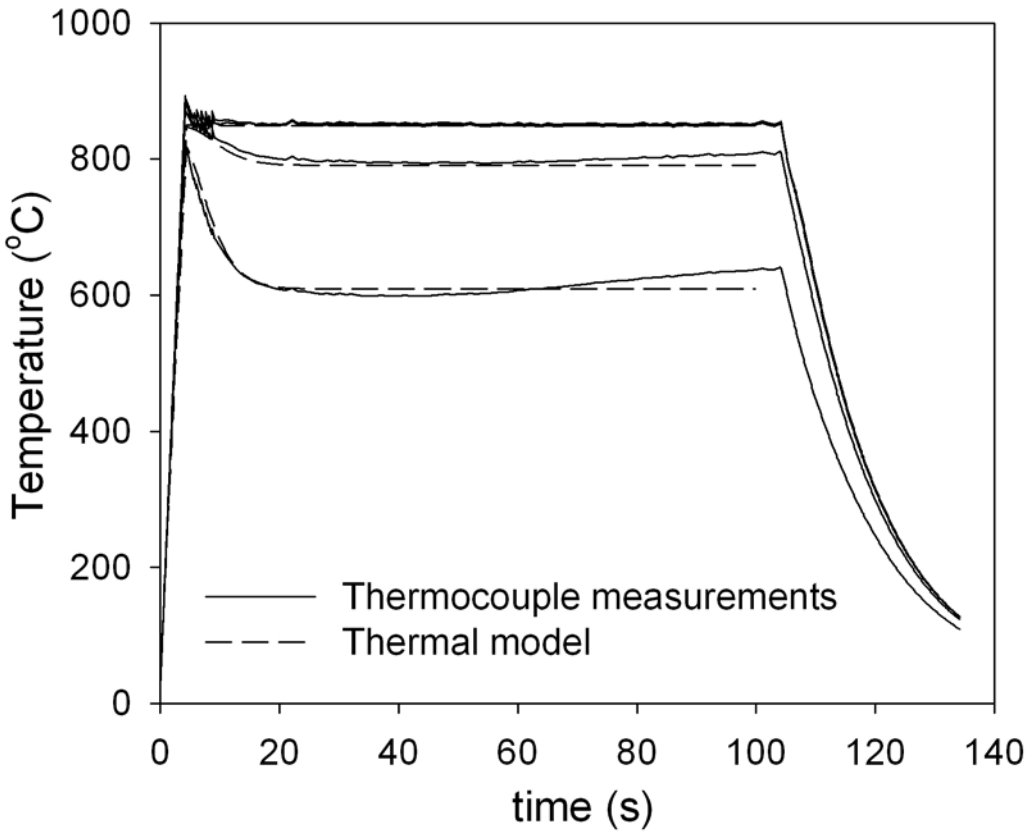
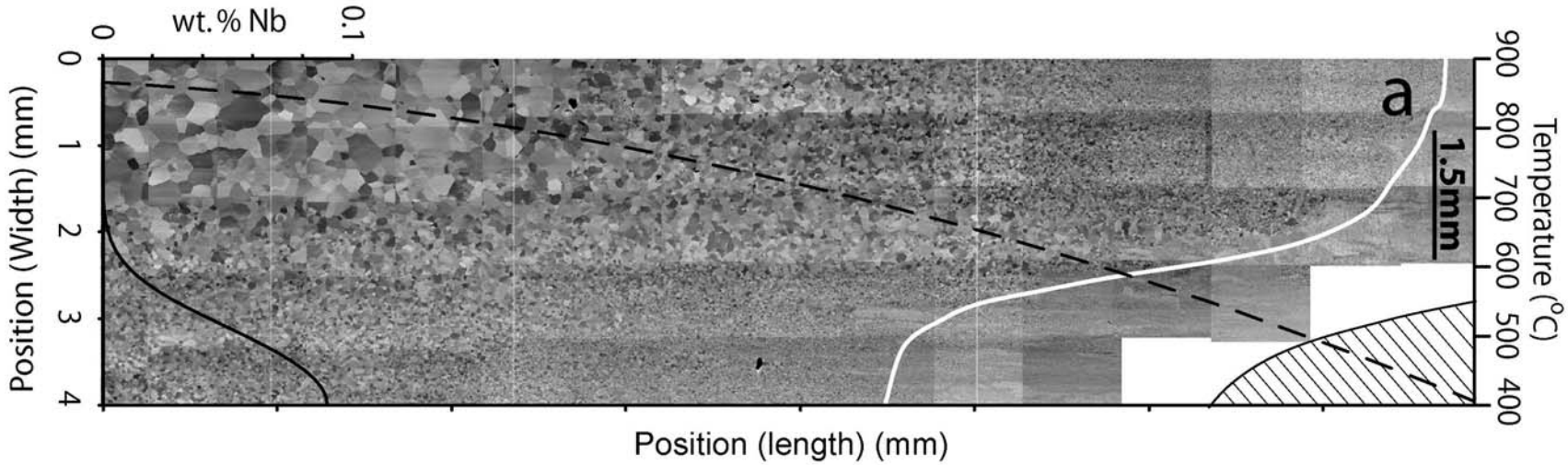
Experimental Set-up is not quite as elegant as we had hoped

→ initial temperature transients are important to incorporate



Nb Solute Effects on Grain Boundary Motion in α

Experimental Results: 100sec Annealing



We should be able to describe the shape of the RXF/No RXF boundary (T, X_{Nb}) and the α grain size as a function of T and X_{Nb}

Nb Solute Effects on Grain Boundary Motion in α

'Minimalist' Model for Recrystallization and Grain Growth

RXF

$$X_{ext} = N_{\mathrm{Re}\,x}\left[\int_0^t M(X_{Nb},T)\cdot G.dt\right]^3$$

GG

$$\frac{dR}{dt} = \frac{M(X_{Nb},T)\cdot\gamma_{gb}}{R}$$

Boundary Mobility

$$M_{Pure} = \beta\frac{D_{Fe}^{Gb}V_m\delta}{b^2RT}$$

$$M(X_{Nb},T) = \left(\frac{1}{M_{Pure}} + \alpha\cdot X_{Nb}\right)^{-1}$$

$$\alpha = \frac{N_V(kT)^2\delta}{E_b D_{Nb}^{Int}}\left(\sinh\left(\frac{E_b}{kT}\right) - \frac{E_b}{kT}\right)$$

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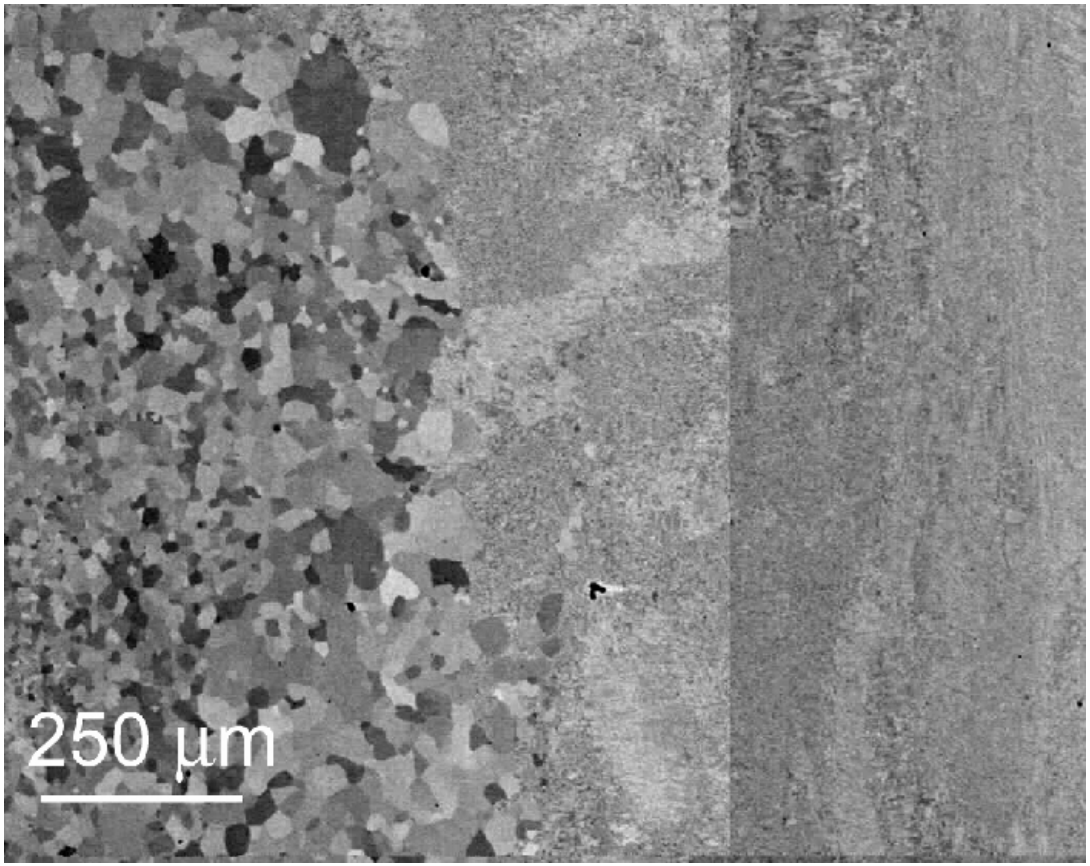
Nucleation of Recrystallization



Assume site saturated nucleation

R_{Nuc}~20µm

$N=5.10^{14}$ m^{-3}

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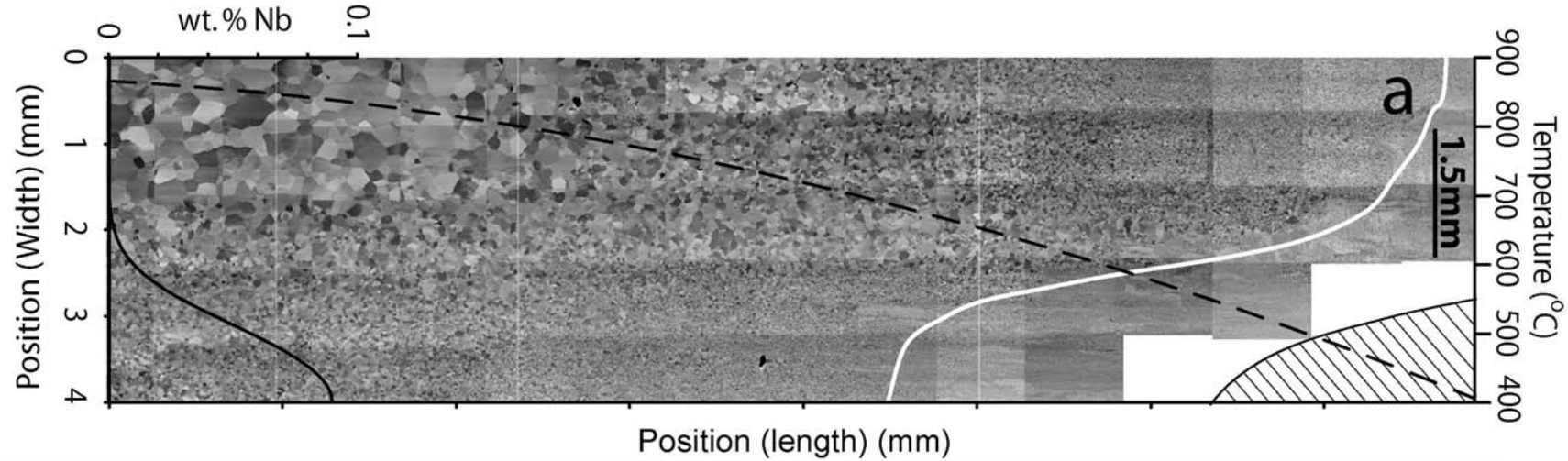
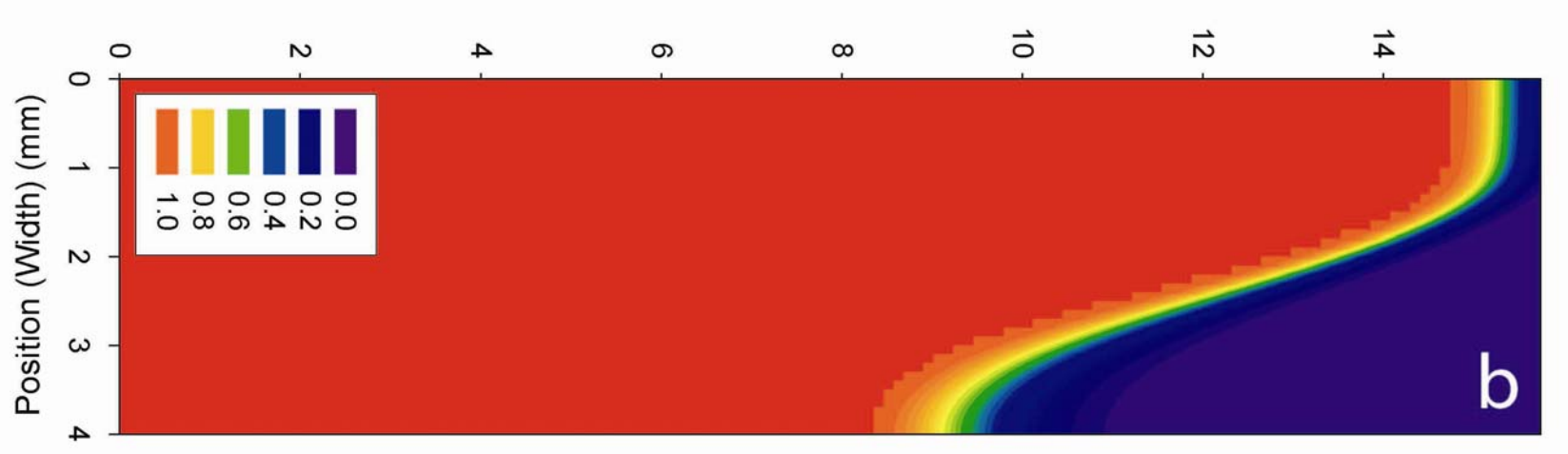
Experimental Results and Model Calculation Comparison





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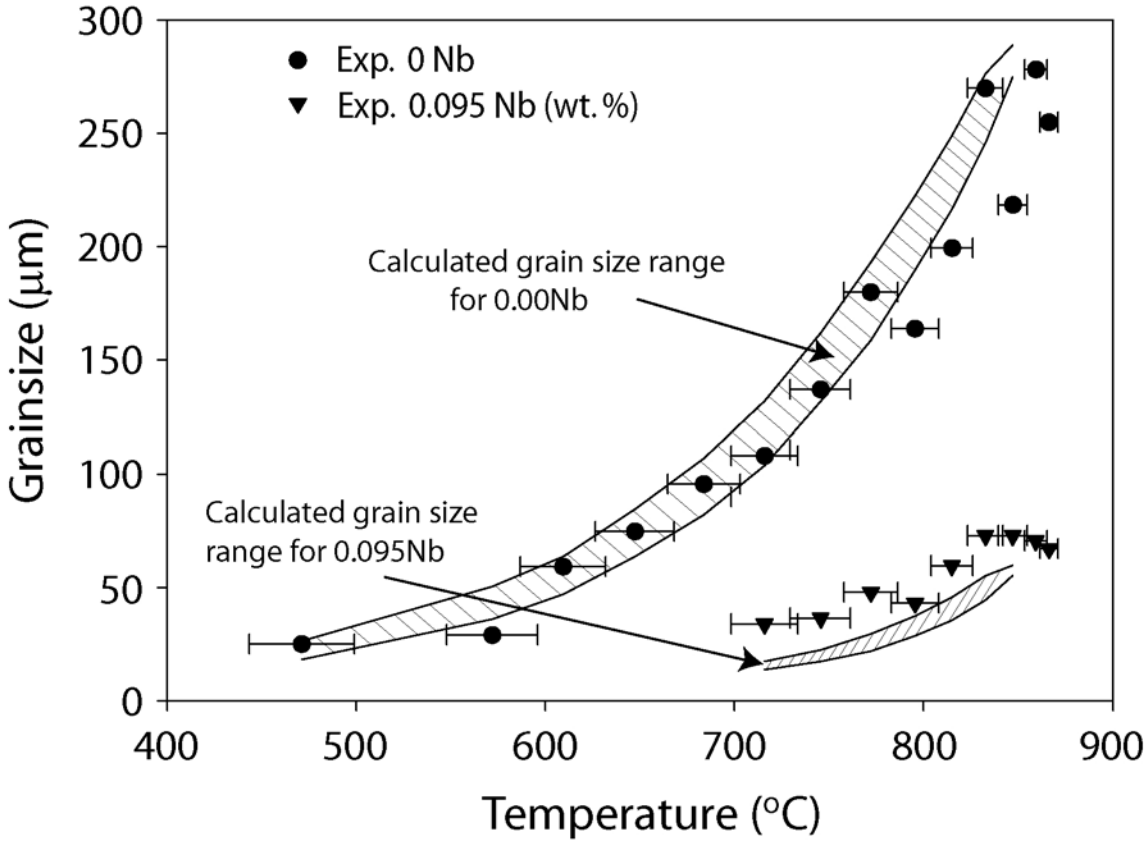

Nb Solute Effects on Grain Boundary Motion in α

Table 1. Values of parameters used in the calculations

Parameter	Value	Ref
δ, grain boundary thickness	$1 \cdot 10^{-9}$ m	-
b, burgers vector in α-Fe	$2.48 \cdot 10^{-10}$ m	
V_m, α-Fe molar volume	$7.09 \cdot 10^{-6}$ m^3	
G, Driving force for recrystallization	1.3 MPa	-
N_{Rex}, Number density of recrystallization nuclei	$5 \cdot 10^{14}$ m^{-3}	-
$D_o^{Fe,Gb}$, Pre-exponential factor for Fe diffusion along grain boundaries in pure α-Fe	$1.5 \cdot 10^{-4}$ m^2/s	[28]
$Q_o^{Fe,Gb}$, Activation energy for Fe diffusion along grain boundaries in pure α-Fe	148 kJ/mol	[28]
β, Turnbull factor	0.7	-
γ, Interfacial energy of α-Fe grain boundaries	0.65	[23-26]
D_o^{Nb}, Pre-exponential factor for Nb diffusion in bulk α-Fe	$3.15 \cdot 10^{-4}$ m^2/s	[28]
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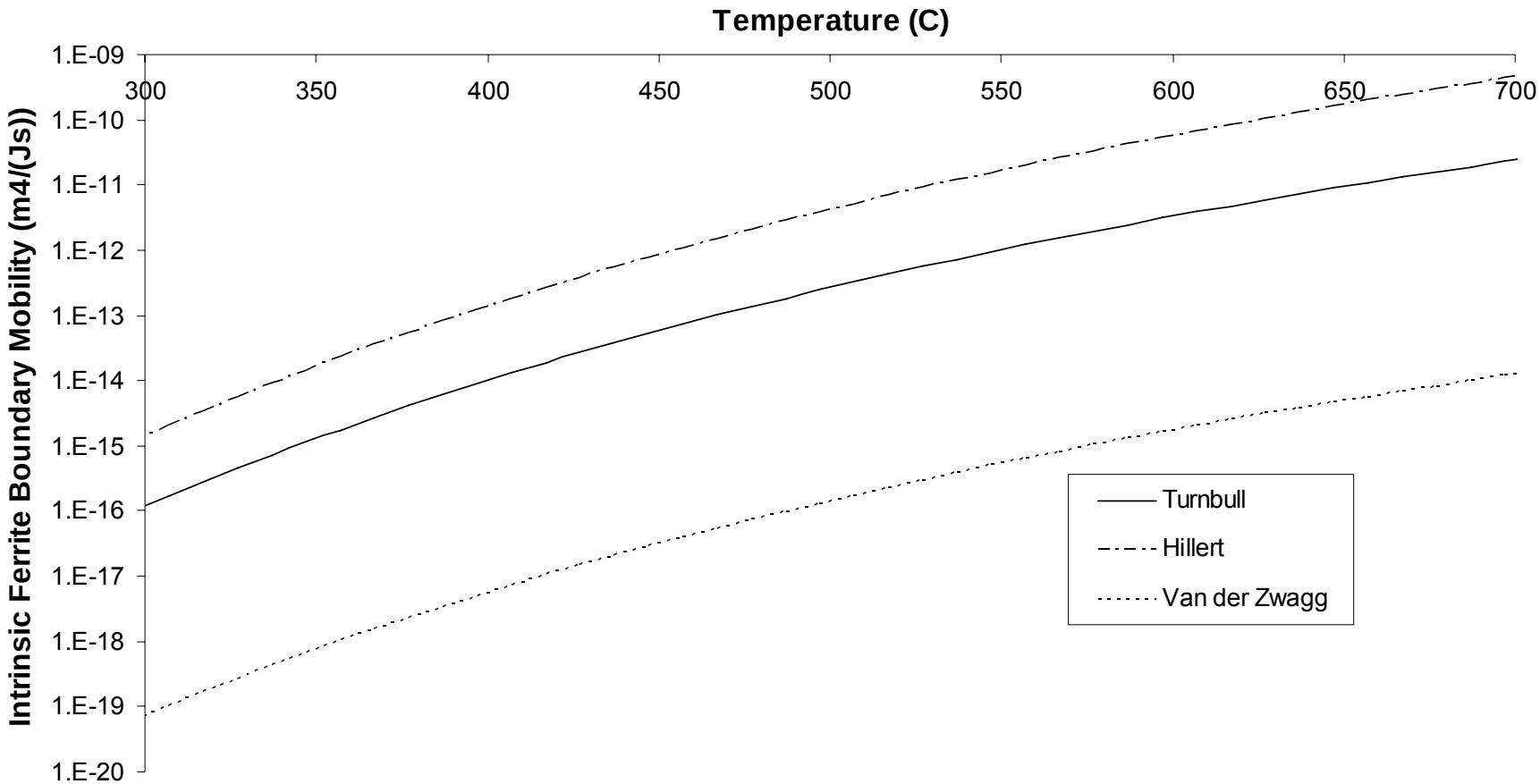
φ, Multiplicative factor for cross-boundary diffusion of Nb	15.0	-
E_b, Nb binding energy to α-Fe grain boundaries	28.9 kJ/mol	[29-30]

A fraction of Turnbull's mobility seems a very good estimate of intrinsic gb mobility

Intrinsic Grain Boundary Mobility in α



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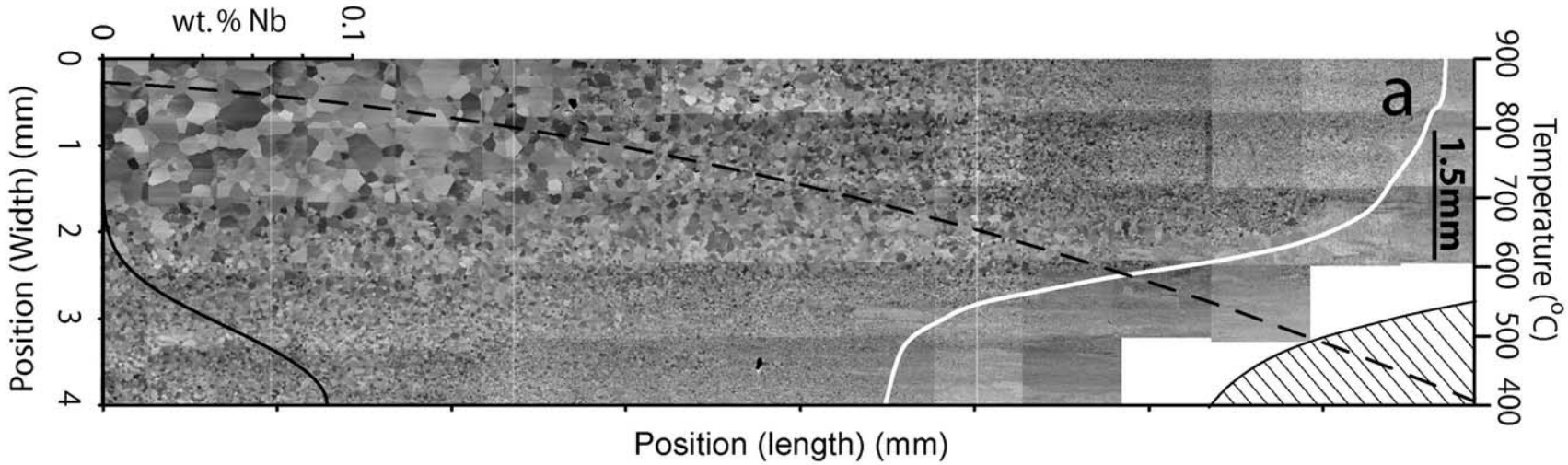

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Nb Binding Energy to Ferrite Grain Boundaries

Maruyama, Smith and Cerezo, Mat. Sci and Eng, 2003, 253, p.126.

Fe-0.087Nb (at. %) 800C

APFIM measured interfacial excess, $\Gamma^s = 9.7 \pm 2.4 \cdot 10^{17}\ atoms/m^2$

→ using a wedge shaped interface profile of width 1nm gives E_b=28.9 kJ/mol

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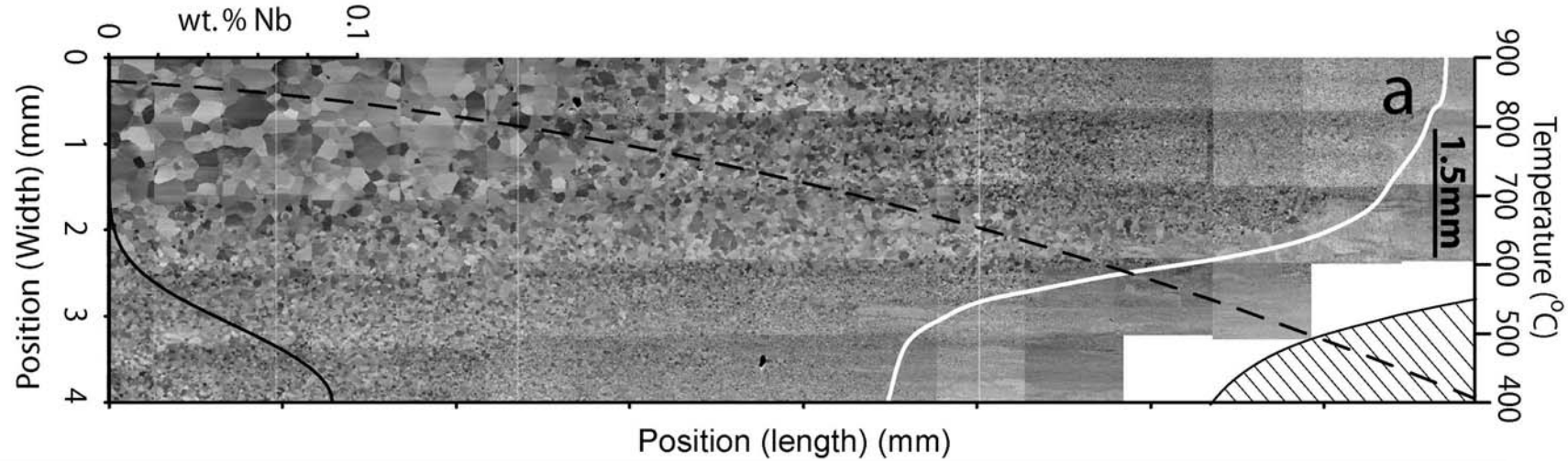

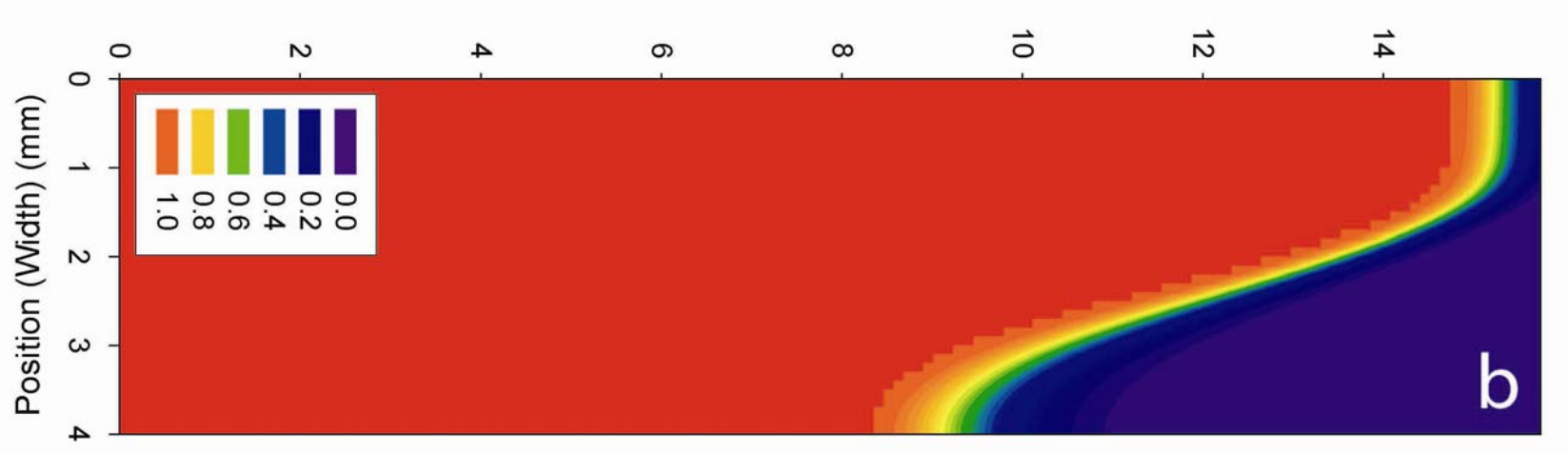

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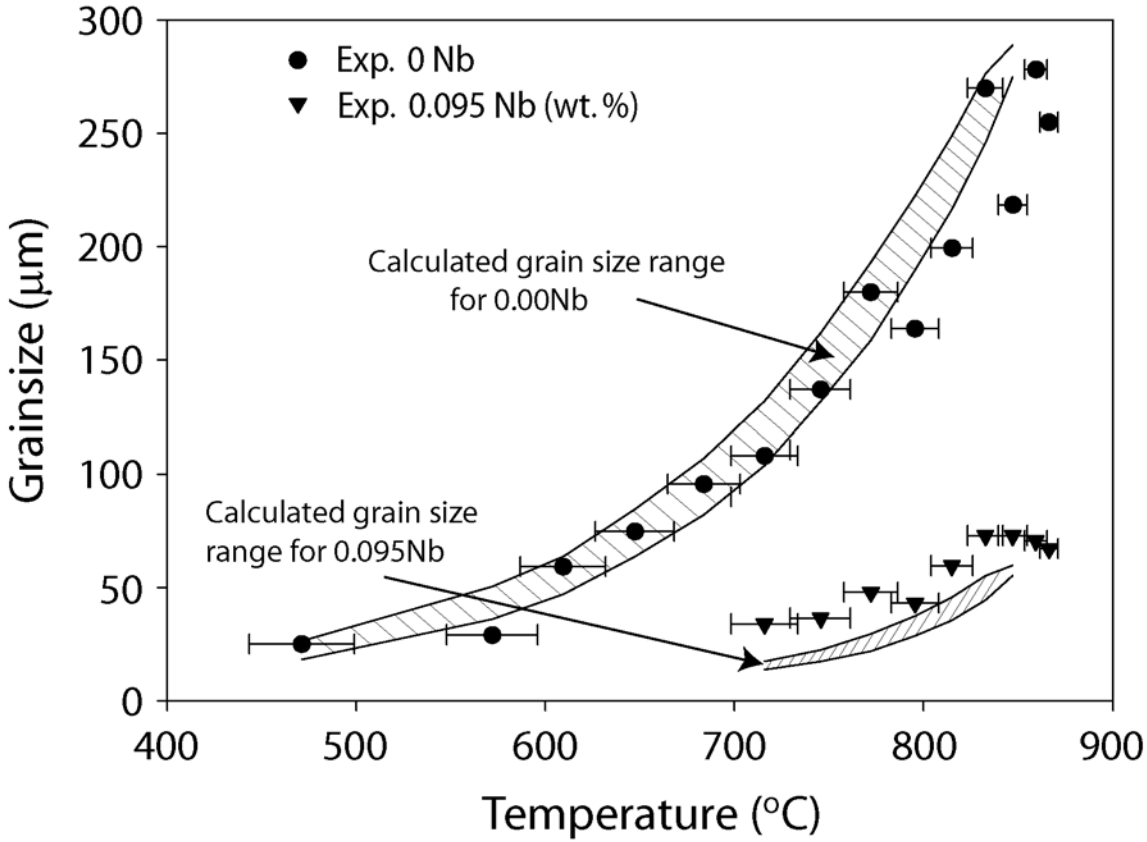

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The trans-interface Nb mobility is only ~15x the bulk α value

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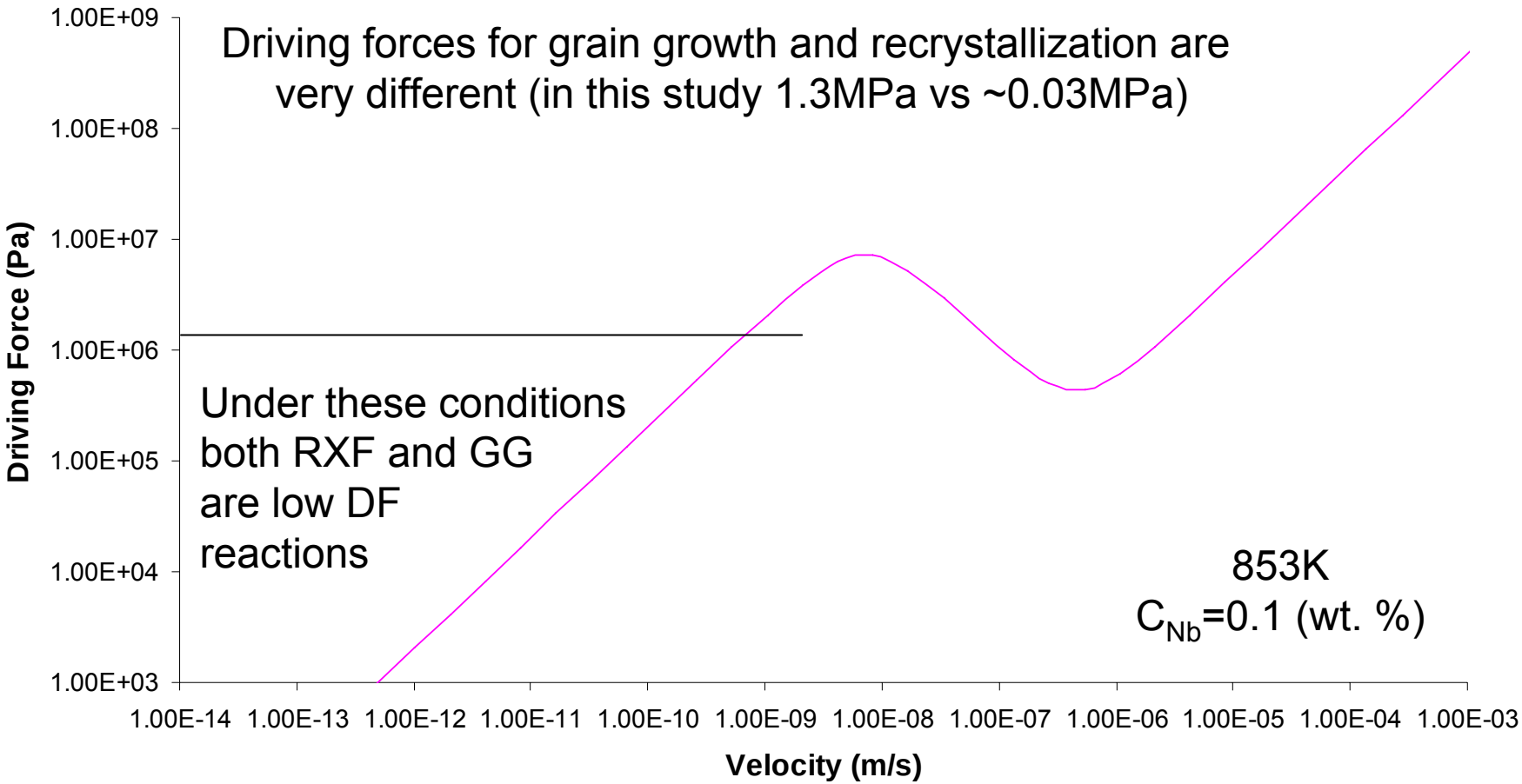

Conclusions

- Combinatorial approaches can be useful for extracting important parameters over significant T and X ranges
- Turnbull mobility seems a good estimate of the grain boundary mobility (the activation energy is that for diffusion along the grain boundary)
- Trans-interface solute mobility is more closely related to the bulk diffusivity (for Nb ~15x diffusivity in α)
- For typical Nb concentrations in microalloyed steels, both recrystallization and grain growth should be considered low DF reactions (they occur in the slow branch of Cahn's SD curve)