CCC Annual Report

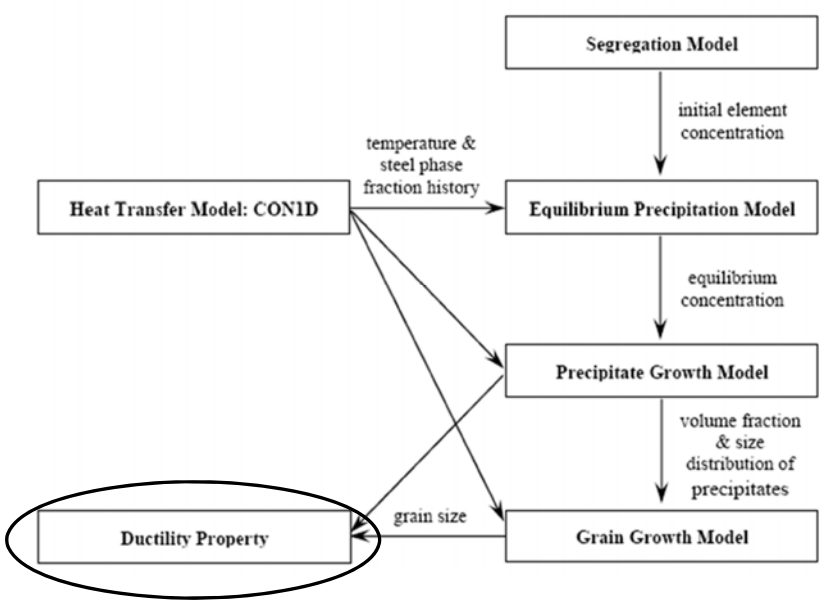
UIUC, August 20, 2014

Thermal Stress Analysis of columnar microstructures and intergranular crack formation

Aravind Murali

Department of Mechanical Science & Engineering
University of Illinois at Urbana-Champaign

Project Overview



Final goal: Design casting practices to prevent transverse cracks

Interplay of phenomena leading to hot ductility and crack formation

Heat Transfer → Micro-structure ←
- Grain Size
- Grain boundary evolution
- Precipitates
- Phase orientations

Micro-structure → Surface & Internal Cracks ← **Metallurgical Embrittlement**

Tensile Stress → Surface & Internal Cracks

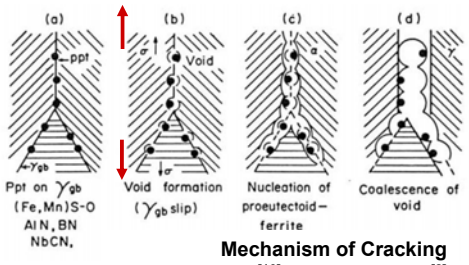
- Temperature Gradients
- Ferro-static Pressure
- Creep bulging (support rolls)
- Friction of shell (against mold)
- Roll Misalignments

Metallurgical Embrittlement →
- High Temp. Solidus-1340˚C → Hot Tearing
- Intermediate Temp. 1100˚C-750˚C → **Intermediate Ductility**
- Low Temp. 700˚C-900˚C

Hot Tearing
- Liquid film due to segregation of residual elements at grain boundary

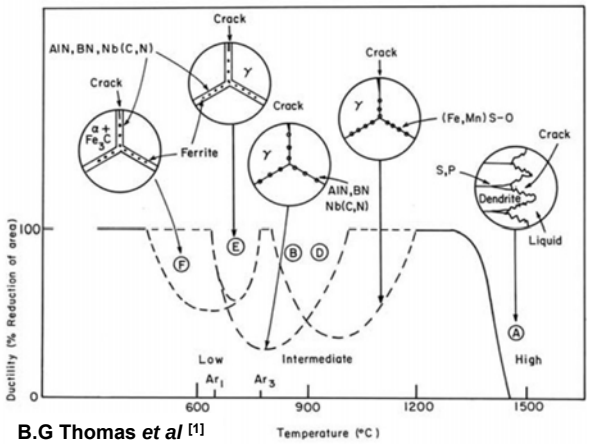
Intermediate Ductility
- Strain concentration at grain boundary ferrite / networks
- Made worse by large grains and fine precipitates

Current work focus



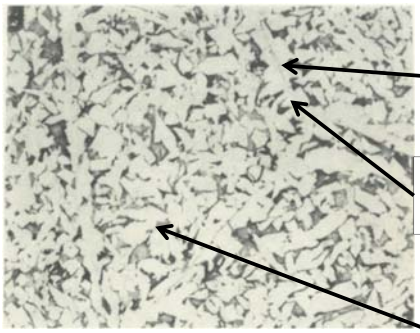
Mechanism of Cracking
Suzuki[10] & Thomas *et al*[2]

Role of Ferrite films in Intermediate Hot Ductility



B.G Thomas *et al* [1]

Current work –Ferrite films on prior austenite grain boundaries



Prior Austenite Grain Boundary

Pro-Eutectoid Ferrite "films"

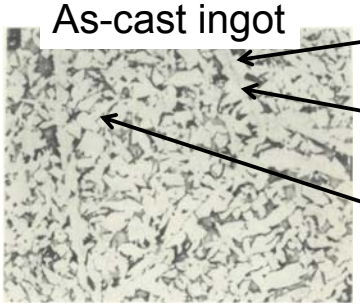
Matrix of austenite and ferrite grains

Source :BG Thomas, PhD Thesis, Fig. 9.6
2% nitol etch [5]

Hypo-eutectoid steel (%C<0.76), cooled below Ar3 → Pro-eutectoid α-Ferrite forms at prior austenite grain boundaries (ferrite films: ~10μm to 30μm thick) → Ferrite is softer (also weakened by precipitation) → Easy crack formation and reduction in ductility (900˚C to 750˚C)

Microstructures of steel with cracks

As-cast ingot

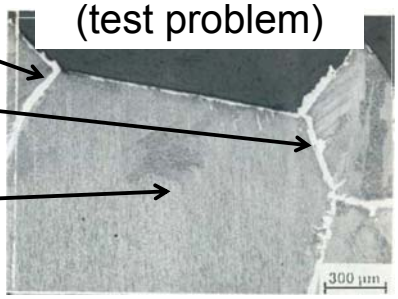


Prior Austenite Grain Boundary

Pro-Eutectoid Ferrite films

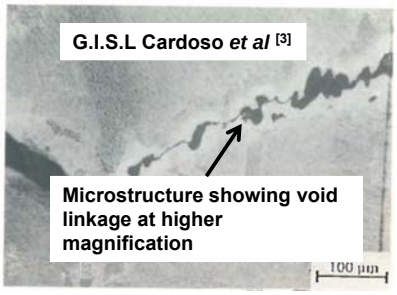
Grain matrix of austenite and ferrite

tensile specimen (test problem)

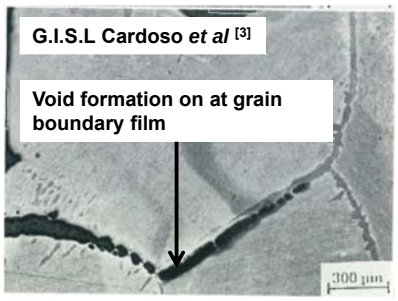


Typical Microstructure expected in Ar3-Ar1 temperature range
BG Thomas, PhD Thesis, Fig. 9.6 [5]

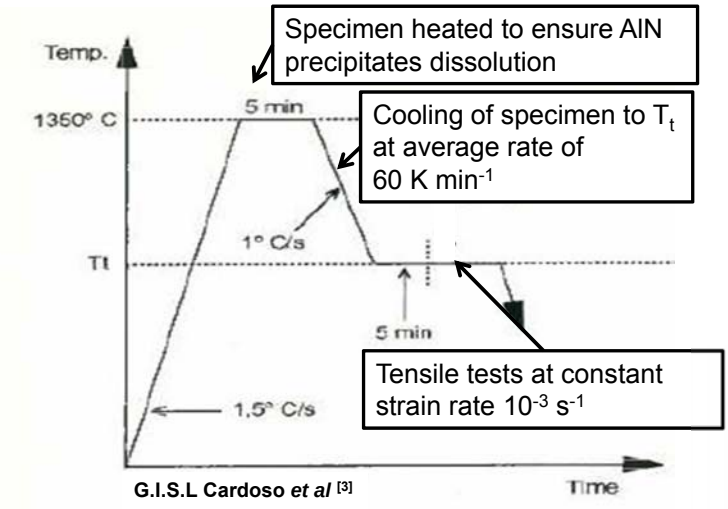
Micro-structure of high Al steel tested at 800C (experiment) shows inter-granular failure associated with ferrite films [3]



Close Up view



Test experiment: measuring hot ductility with ferrite films[3]



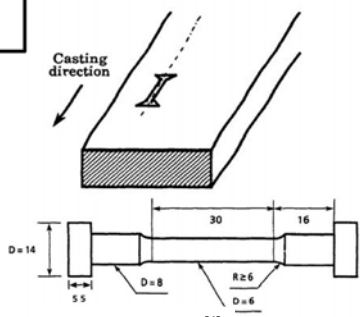
G.I.S.L Cardoso *et al* [3]

Steel grade – High Al steel

Element	Composition (%wt)
Carbon	0.079
Manganese	0.40
Silicon	0.019
Phosphorous	0.006
Sulfur	0.008
Aluminum	0.085
Nitrogen	0.0050

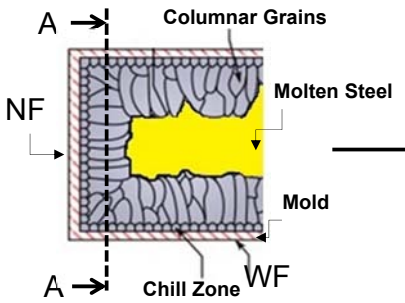
Grain details	Size (unit)
Grain size	460µm[4]
Ferrite film thickness	30µm[4]

Expt detail	Value (unit)
Temperature	800˚C[4]
Strain rate	$1x10^{-3}$[4]

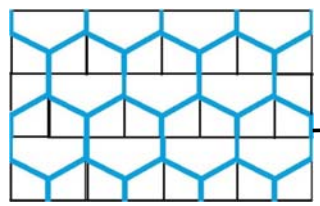


G.I.S.L Cardoso [4]

Simulation domain from columnar zone in cast slab

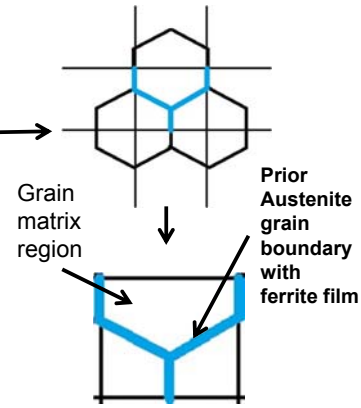


Cross-section of cast slab[6]



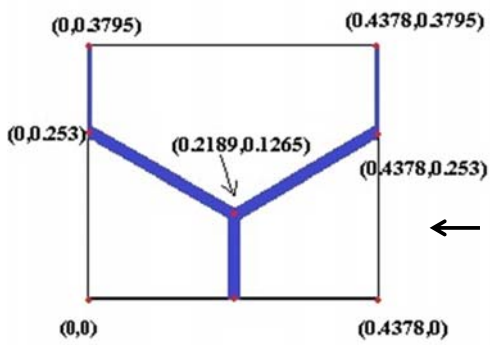
Left section view AA'

Honeycomb cross-sectional structure of regular hexagonal columnar grains into the plane



The unit cell must remain periodic so that the fundamental repeating character is maintained

Grain size of 460μm (test experiment), Dimensions of a regular hexagon with same area (see next slide)



Relating Grain boundary side lengths with grain size measurements

Test experiment grain size is **460μm**

Equivalent Area Principle

Assume d=grain size

a is side of hexagon-shaped grain is related to d:

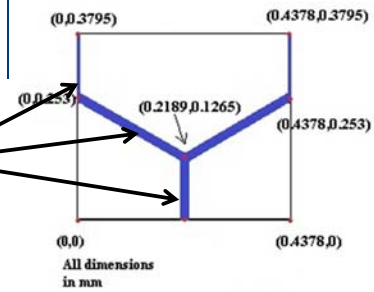
$$a = \sqrt{\frac{d^2 \times \pi}{6\sqrt{3}}} = 0.2529mm$$

Arranging grains in a regular hexagon such that there are equal length of grains along the three grain boundaries and the triple point is located close to the center of the domain

Other geometric properties of a hexagonal grain:

In-radius = $\frac{a \times \sqrt{3}}{2}$=0.219mm

Circumradius = a=0.2529mm



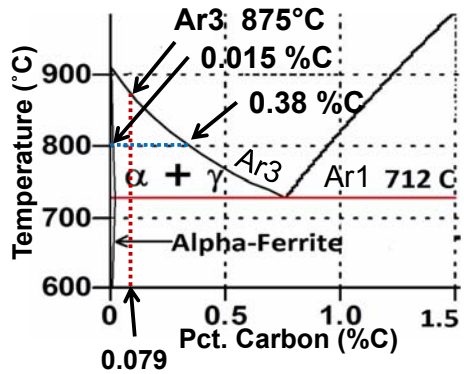
ASTM Standard

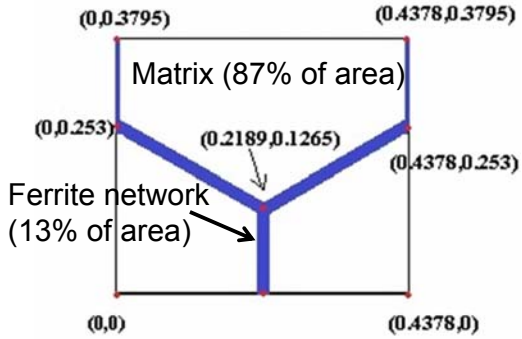
Since 1 grain is present in an area of 0.1661mm^2

Grain number is 6.02 grains/mm^2

From ASTM handbook, 1948 ed., grain number of 6 corresponds to a grain diameter of ~0.425mm (ASTM Grain number between -1 and 0)

Phase &microstructure fractions for Matrix and Grain Boundary





Total Area of domain = 0.166mm^2
(See Appendix 3 - %Wt. = %Volume)

Phase fractions from Fe-C phase diagram[9] lever rule-

$$\%w_{ferrite} = \frac{0.38 - 0.079}{0.38 - 0.015} = 82\%$$

$$\%w_{austenite} = \frac{0.079 - 0.015}{0.38 - 0.015} = 18\%$$

Matrix (87%)	Ferrite (13%)
80% ferrite (v_{fer}) @ 0.015%C	100% ferrite @ 0.015%C
20% austenite (v_{aus}) @ 0.38% C	

Results: Microstructure is:

- grain boundary ferrite network of 100% alpha ferrite (assumed)
- matrix of **80% ferrite** & **20% austenite**

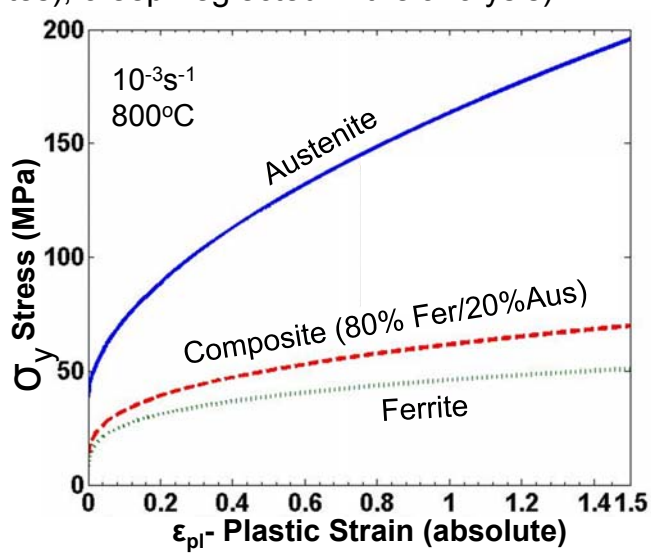
Total ferrite in domain $= 0.8 \times 0.87 + 1 \times 0.13 \sim 0.82$
Total austenite in domain $= (1 - 0.82) \sim 0.18$

Total %C = 0.18x0.38+0.82*0.015= **0.08%C**

Mechanical Properties (E & σ_y) for Grain Matrix and Grain Boundary

An elastic - plastic model for mechanical behavior is used.
(The time scales are small (in minutes), creep neglected in the analysis)

Property	Value
Elastic modulus of ferrite film	95000 MPa [13]
Poisson Ratio of ferrite film	0.3 [13]
Elastic modulus of Grain Matrix	95000 MPa [13]
Poisson ratio of Grain Matrix	0.3 [13]
Plastic strength of ferrite film	Zhu model for Ferrite [11]
Plastic strength of Grain Matrix	Austenite-Kozlowski[12] & Ferrite - Zhu[11]



The composite grain properties using fiber-composite equations (next slide)

Composite-Grain Matrix σ_y- ε_{pl} calculation

Use equations of particle reinforced composites
(See W. Callister, Mat. Sci and Engg (7th Edition), p585 [2]

$$\sigma_{upper} = \sigma_{aus} V_{aus} + \sigma_{fer} V_{fer}$$

$$\sigma_{lower} = \frac{\sigma_{aus} \times \sigma_{fer}}{V_{aus} \times \sigma_{ferrite} + V_{fer} \times \sigma_{aus}}$$

$$\sigma_{average} = \frac{\sigma_{lower} + \sigma_{upper}}{2}$$

σ_{aus} – **Strength of austenite phase,**
σ_{fer} – **Strength of ferrite phase**
V_{aus} – **Volume fraction of austenite**
V_{fer} – **Volume fraction of ferrite**

$\sigma_{average}$ **is used for stress-strain property of grain matrix in model**

GTN model for Grain Model: based on Porous Metal Plasticity

The Gurson-Tvergaard-Needleman[6] model predicts ductile fracture due to void nucleation and growth. In ABAQUS it is implemented as Porous Metal Plasticity Model[7]

Yield condition given as $\phi = \left(\frac{q}{\sigma_y}\right)^2 + 2q_1 f \cosh\left(-\frac{3}{2}\frac{q_2 p}{\sigma_y}\right) - (1 + q_3 f^2) = 0$

$$\dot{f} = \dot{f}_{gr} + \dot{f}_{nucl}$$

$$\dot{f}_{gr} = (1 - f)\,\dot{\boldsymbol{\varepsilon}}^{pl} : \mathbf{I}$$

$$\dot{f}_{nucl} = A\,\dot{\bar{\varepsilon}}_m^{pl}$$

$$A = \frac{f_N}{s_N\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\bar{\varepsilon}_m^{pl} - \varepsilon_N}{s_N}\right)^2\right]$$

- Total rate of change of Void fraction ($\dot{f}$)
- Rate of change of Void fraction due to void growth ($\dot{f}_g$)
- Rate of change of Void fraction due to void nucleation ($\dot{f}_n$)
- deviatoric stress (q)
- hydrostatic pressure (p)

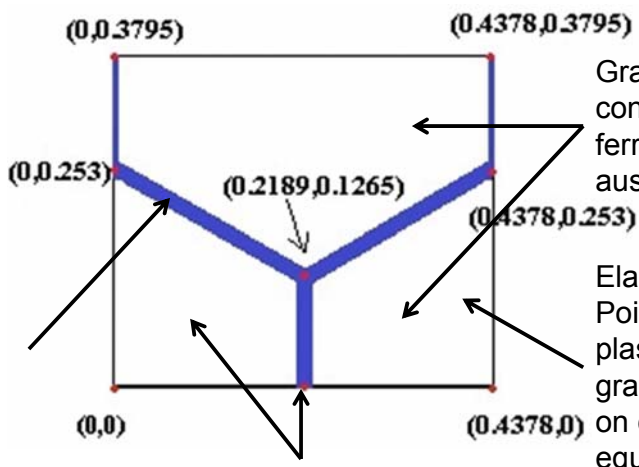
At Grain Matrix

Parameter	Value [9][7]
q1	1.5
q2	1.0
q3	2.25
Initial void fraction, f_0	0.005
Void nucleation Distribution	ε_N0.3/S_N 0.1
Volume fraction of nucleated voids, f_N	**0.004**

At Grain Boundary

Parameter	Value[8][7]
q1	1.5
q2	1.0
q3	2.25
Initial void fraction, f_0	0.005
Void nucleation Distribution	ε_N 0.3/S_N 0.1
Volume fraction of nucleated voids, f_N	**0.04**

Grain model – complete description



Grain matrix consists of 80% ferrite and 20% austenite

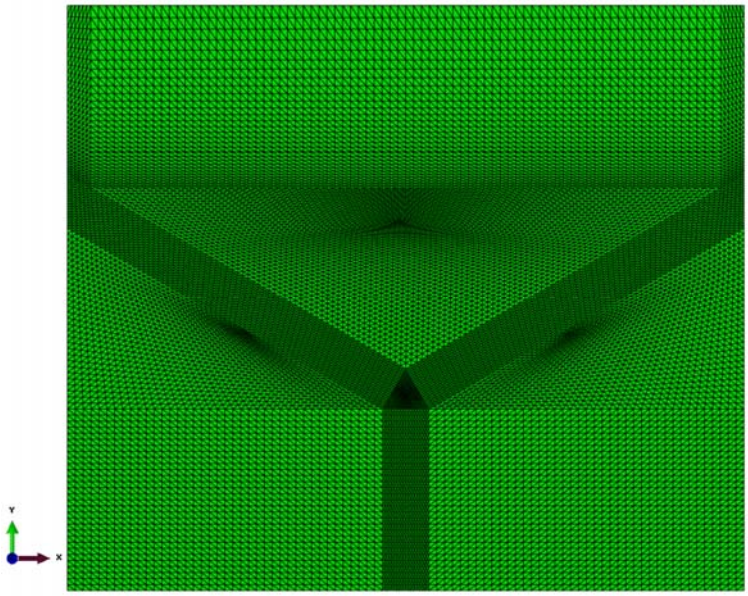
Grain boundary consists of 100% ferrite film

Elastic modulus, Poisson ratio and plastic strength of ferrite (Zhu model [11])

Elastic modulus, Poisson ratio and plastic strength of grain matrix based on composite equations

The GTN model is used for ductile fracture in <u>both grain matrix and grain boundary region</u>

Grain model: Unit Cell Domain Mesh Details

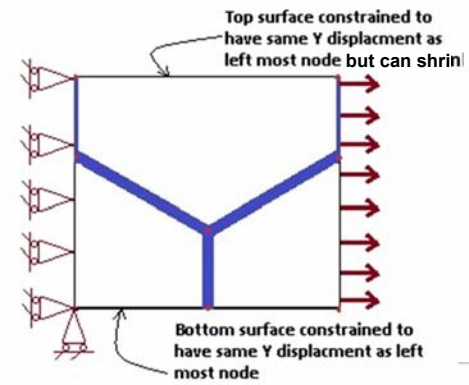


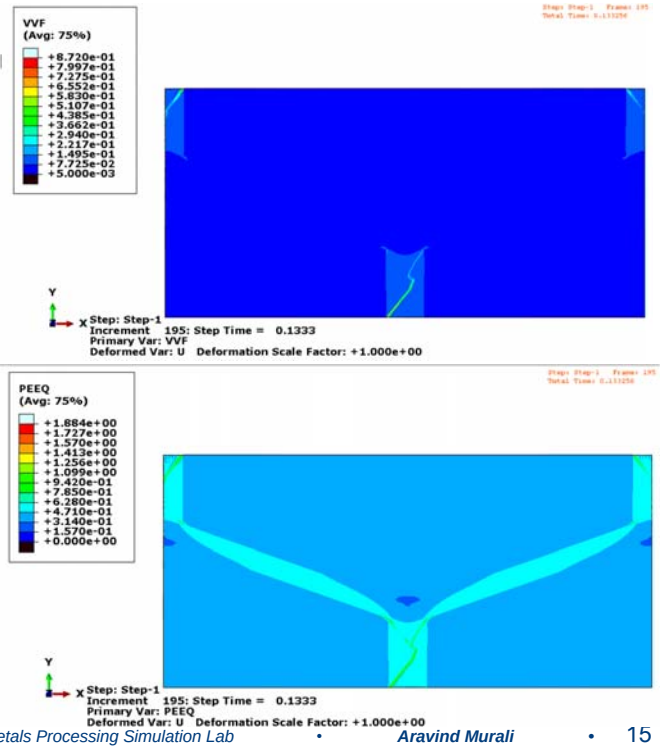
Mesh created in ABAQUS 6.13-2

Number of nodes: 57078
Number of elements: 28332
Element types: CPEG6H

Typical wall clock time of around 7000seconds on 3 Intel Xeon processors (1.8Ghz)

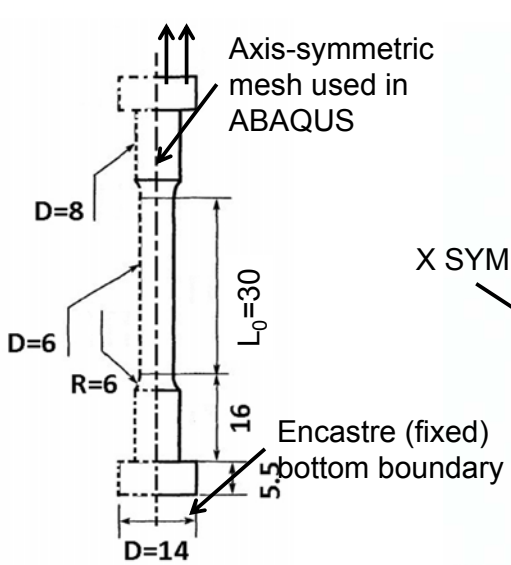
Grain Model Case 1 – Unit cell strained along horizontal axis

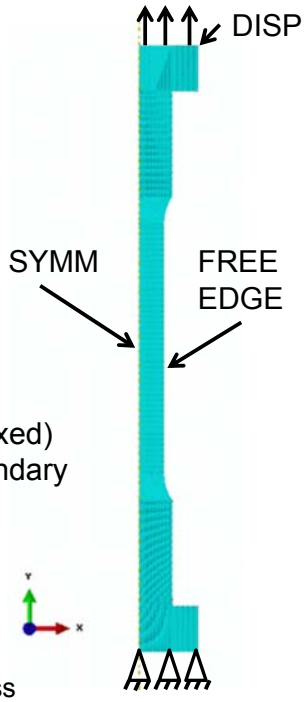




1. Right domain boundary is displaced right until failure
2. Max stress reached at 0.39 macro plastic strain (0.46 total macro-strain)
3. More plastic strain on softer grain boundaries
4. Strain concentration on grain boundary leads to failure

Axis-symmetric Tensile Specimen domain





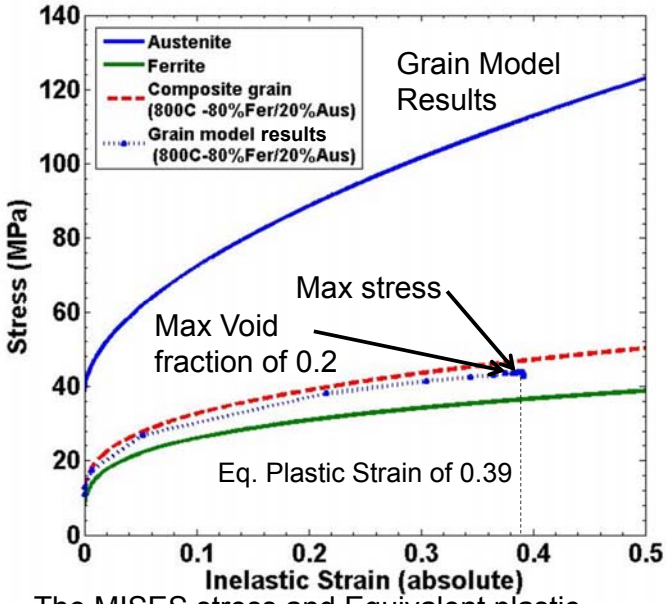
Details of mesh
- 136501 nodes
- 135000 quadrilateral elements
- CAX4R elements used

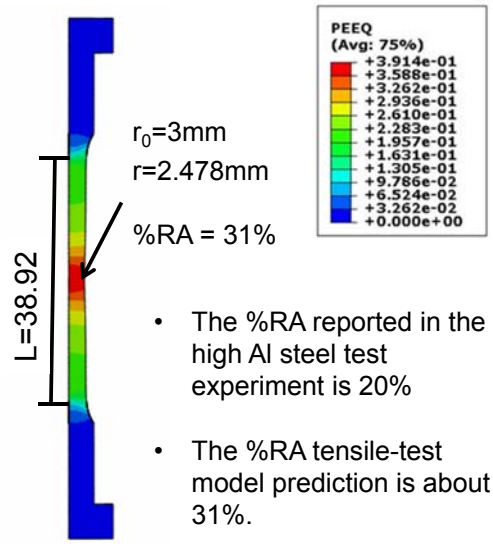
Properties Used
- Properties are same as input to grain model except:
- Plastic stress-inelastic strain behavior from grain-model results

ABAQUS Step size
- Smallest step = 1×10^{-9}s
  - Largest step = 1s

$\varepsilon_{tr} = \ln(1+\varepsilon_e)$ — ε_{tr}-True strain
$\sigma_{tr} = \sigma_e(1+\varepsilon_e)$ — ε_e-Engineering strain
σ_{tr}-True stress
σ_e-Engineering stress

Tensile-test Macro-Model to compare with test experiment



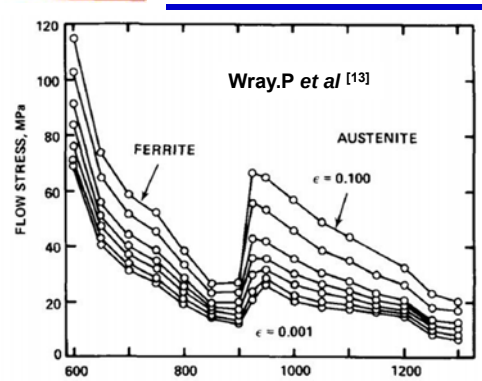


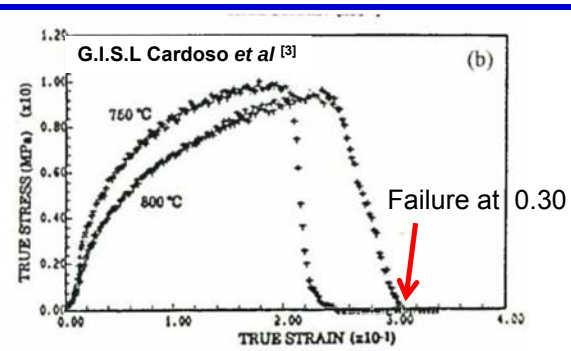
- The %RA reported in the high Al steel test experiment is 20%
- The %RA tensile-test model prediction is about 31%.

The MISES stress and Equivalent plastic Strain is averaged over the entire grain model to obtain the stress-strain relationship, which is then **input into the tensile test model**

Displacement along vertical to cause failure is 8.92mm
29% total macro-strain (engineering strain)

Comparison between experiment[3] and computational model





Measurements of Flow Stress from Peter Wray [13] (basis for strength data of ferrite and austenite) and from Cardoso [3] **do not match**

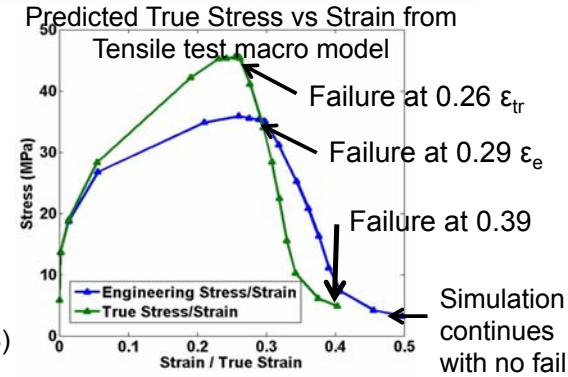
$\varepsilon_{tr} = \ln(1+\varepsilon_e)$ — ε_{tr}-True strain

$\sigma_{tr} = \sigma_e(1+\varepsilon_e)$ — ε_e -Engineering strain

$\varepsilon_e = \frac{L}{L_0}$ — σ_{tr} -True stress

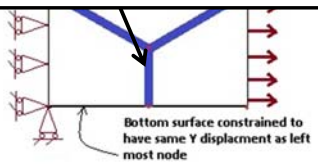
σ_e -Engineering stress (calculated from σ_z in ABAQUS)

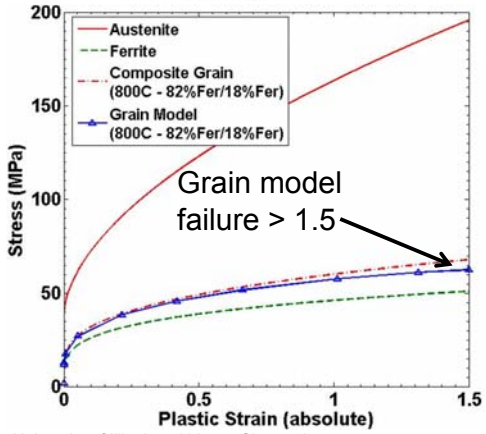
Predicted True Stress vs Strain from Tensile test macro model

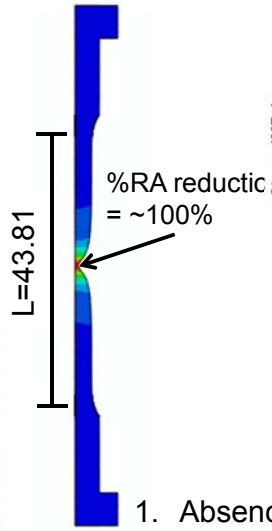


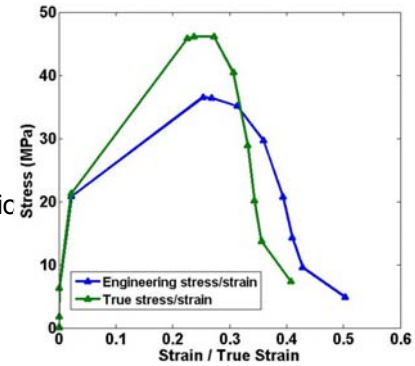
Repeat test experiment with uniform ferrite grain distribution (no ferrite networks)

Strength of grain-boundary region (blue) is assumed equal to strength of composite grain matrix (800ºC – 82%Fer/18%Aus)









Stress vs Strain graph for typical tensile specimen

1. Absence of ferrite films means no strain concentration in grain boundary and no failure
2. The tensile specimen necks till **~100% RA with no embrittlement**

Case 2 - Effect of Temperature

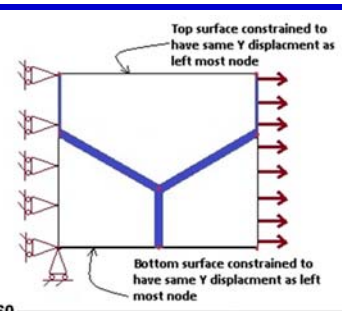
Increasing temperature to 870˚C
(It is at this temperature that ratio of strength of grain matrix to ferrite film is twice the ratio at 800˚C)

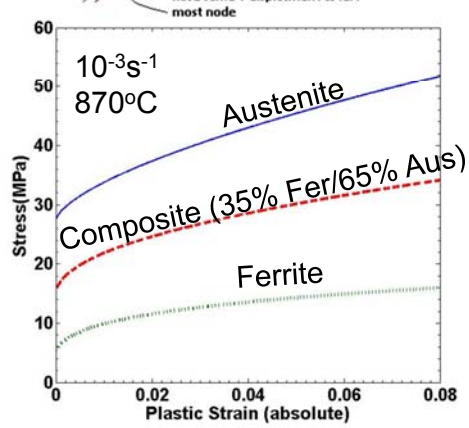
Phase fractions from Fe-C phase diagram[9] lever rule-

$\%w_{ferrite} = 35\%$ $\%w_{austenite} = 65\%$

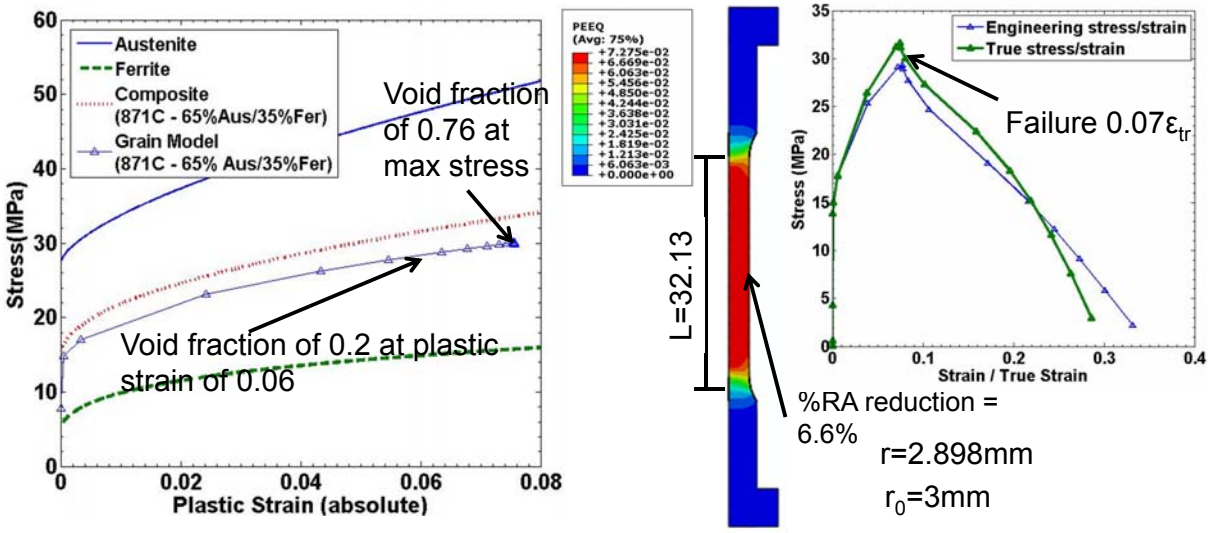
Matrix (87%)	Ferrite (13%)
35% ferrite @ 0.002%C	100% ferrite @ 0.002%C
65% austenite @ 0.12%C	

Elastic modulus =70150 MPa[11]
Poisson Ratio = 0.3
Plastic Strength of ferrite film = Zhu model[11]
Plastic Strength of grain matrix =
Austenite (Kozlowksi)[12] + Ferrite (Zhu Model)[11]





Tensile test Macro-Model for high temperature (870^{0}C) case



There is maximum stress reached in grain domain at 7% applied macro strain
Tensile test for higher temperatures fail at much lower strain (7%) in compared to 29% strain at failure for Tensile test in Case 1

Summary and future work

Summary –

- A micro-structure based methodology is developed to analyze hot ductility of steels using a macro-micro model approach
- Model roughly matches ductility measurements in lab tensile test
- Ferrite networks cause large drop in ductility (as observed) explaining the lower ductility in 2-phase temperature region
- Effect of temperature on ductility matches observations. Decreasing temperature (from 870˚C to 800˚C) increases ductility from 6.6% to 31%

Future Work –

- Void fractions due to precipitates can be studied in combination with other models
- Application to a real world caster with different loading and boundary conditions
- Effect of different grain sizes and ferrite film thicknesses can be investigated

Acknowledgments

- Continuous Casting Consortium Members (ABB, ArcelorMittal, Baosteel, Magnesita Refractories, Nippon Steel and Sumitomo Metal Corp., Nucor Steel, Postech/ Posco, Severstal, SSAB, Tata Steel, ANSYS/ Fluent)
- Dr. Koric, Dr. Lance, Prof. Thomas and other members of my research group

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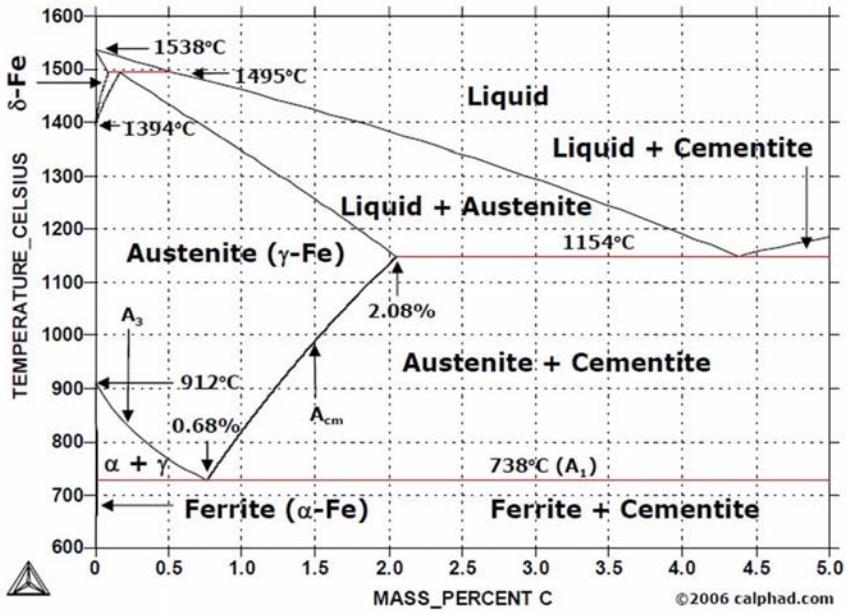
Thank you

Appendix 2 Fe-C Phase diagram

Refer Iron-Carbon phase diagram from www.calphad.com/iron-carbon.html



Appendix 3 – Difference between volume and % weight at 800C for alpha ferrite and austenite[*]

$$\rho_\alpha(\frac{kg}{m^3}) = 7881 - 0.324 \times T(°C) - 3 \times 10^{-5} \times T^2(°C)$$

$$\rho_\gamma(\frac{kg}{m^3}) = \frac{100 \times (8106 - 0.51 \times T(°C)}{(100 - (pct\ C)) \times \left(1 + 0.008 \times (pct\ C)\right)^3}$$

Since the temperature is known (from experiment), we use 800°C

$$\rho_\alpha(\frac{kg}{m^3}) = 7881 - 0.324 \times 800 - 3 \times 10^{-5} \times 800^2 = 7602.6\ (\frac{kg}{m^3})$$

$$\rho_\gamma\left(\frac{kg}{m^3}\right) = \frac{100 \times (8106 - 0.51 \times 800)}{\left(100 - (0.079)\right) \times \left(1 + 0.008 \times (0.079)\right)^3} = 7689.58(\frac{kg}{m^3})$$

For a ferrite volume fraction of 82%, the corresponding wt. fraction of ferrite corresponds to-

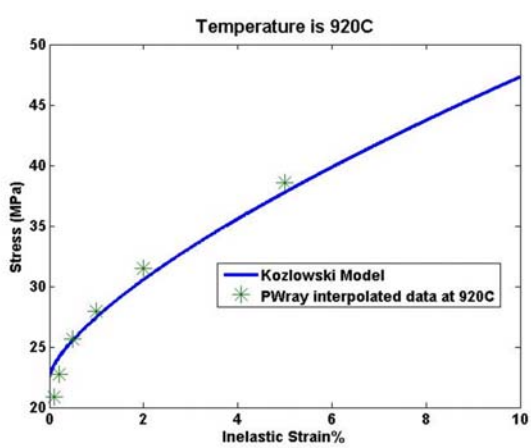
$$\%wt_\alpha = \frac{0.82 \times 7602.6}{0.18 \times 7689.58 + 0.82 \times 7602.6} = 81.8\%$$

Since a the %wt fraction of ferrite is almost the same as volume fraction, we can take volume fraction of ferrite and avoid this calculation

[*] – Li, Chunsheng and Thomas, BG, "Thermomechanical Finite-Element Model of Shell Behavior in Continuous Casting of Steel", Metallurgical and Materials Transactions B, Vol.35B, December 2004 – pg.1151-1172

Appendix-4 :Comparison of Kozlowski model and Wray's[*] data at 920°C

Carbon Content – 0.005% and strain rate $1 \times 10^{-3} s^{-1}$

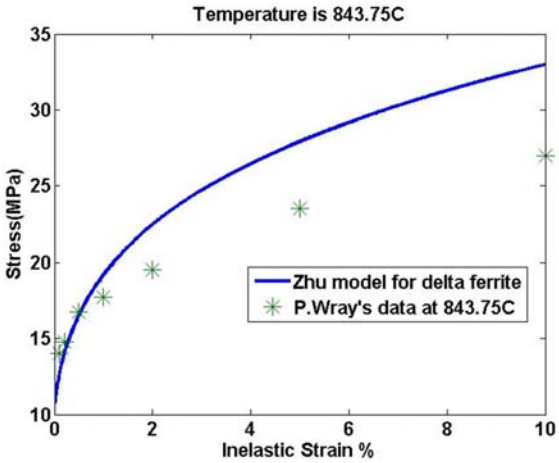


- 920C is above the temperature for start of austenite to ferrite transformation – 912C
- At this temperature, the microstructure should consist of Austenite only
- Hence this data from experiments by P.Wray (for a similar %C) are compared with the Kozlowksi model at this temperature to verify the validity of using these properties
- P.Wray's extrapolated data matches well with the Kozlowski model for Austenite at this temperature

[*] Wray, P.J. "Effect of Carbon Content on the Plastic Flow of Plain Carbon Steels at Elevated Temperatures." Metallurgical Transactions A, Vol. 13A, January 1982,Pg.125-134

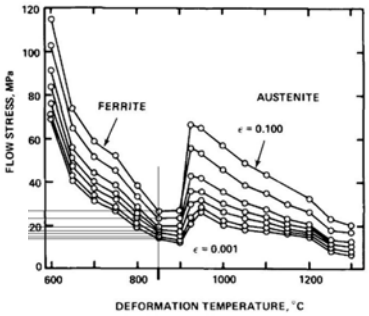
Appendix 4: Comparison of Zhu model and Wray's[*] data at 845°C

Carbon Content – 0.007% and strain rate $2.3 \times 10^{-2} s^{-1}$



- Comparing Zhu's model for delta ferrite with P. Wray's data for 0.007%C steel at 845˚C
- At this temperature and this carbon content, the phase is predominantly Alpha Ferrite.
- Hence a comparison can be made with the Zhu model

P.Wray original figure used for comparison



RMS error between
Wray's data and Zhu's model = 1.18 MPa

[*] Wray, P.J. "High Temperature Plastic-Flow Behavior of Mixtures of Austenite, Cementite, Ferrite, and Pearlite in Plain-Carbon Steels" Metallurgical Transactions A, Vol. 15A, November 1984,Pg.2041-2058