GREAT DESIGNS IN STEEL

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GREAT DESIGNS IN STEEL

NON-EQUILIBRIUM THERMODYNAMIC MODELING TO AID MATERIALS DESIGN FOR QUENCH AND PARTITION (Q&P) STEELS

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[1]QuesTek Innovations LLC, [2]Northwestern University

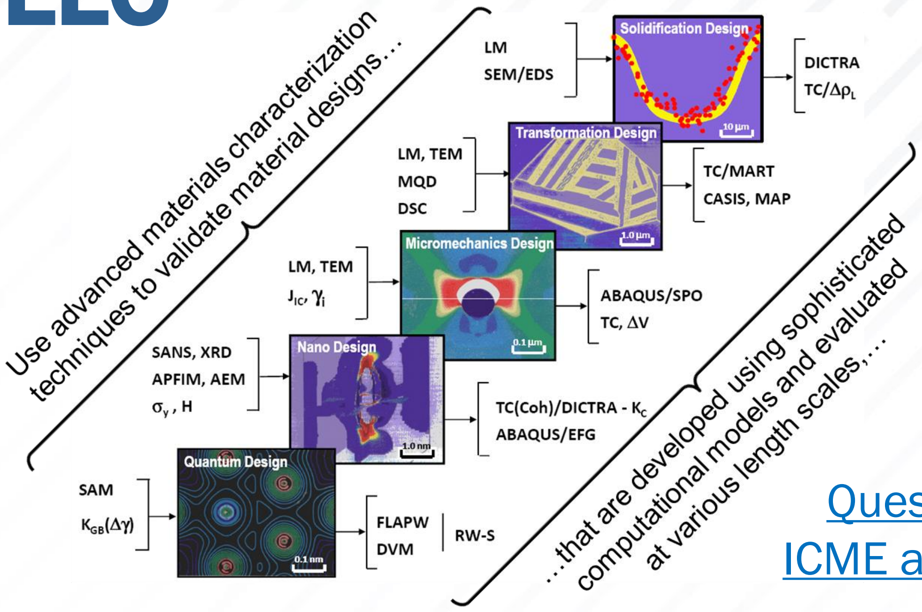
TALK OUTLINE

- Introduction to QuesTek Innovations LLC
- Background of 3rd Gen AHSS and Q&P steels
- Design approach and Flowchart
- Influence of Q&P processing parameters
- Thermodynamic models development and validation
- Design of Q&P steels using developed ICME models
- Summary and ongoing efforts at QuesTek related to AHSS

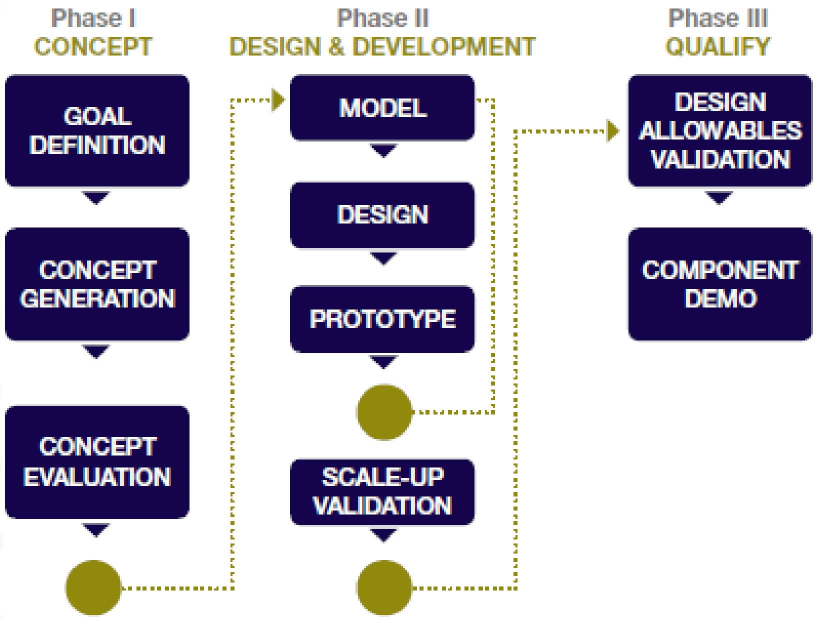
QUESTEK INNOVATIONS LLC

GDIS

- Global leader in **computational materials design**, property modeling and chemistry/process optimization
- QuesTek **ICME approach** applied for design/deployment of novel materials for government and industrial sectors
- Materials designs and property modeling expertise in casting, forging and Additive Manufacturing, and subsequent HIPing and heat treatment processes
- **Systems-based design approach** utilizing computational tools to model key process-structure and structure-property linkages
- Replacing the legacy trial-and-error approaches with parametric materials design



QuesTek's ICME approach



QUESTEK DEVELOPED MATERIALS

- ICME Designed Steel for Aerospace applications

<u>Ferrium® S53® structural steel</u>

USAF landing gear, flight-critical space components

From material design to flight in 10 years

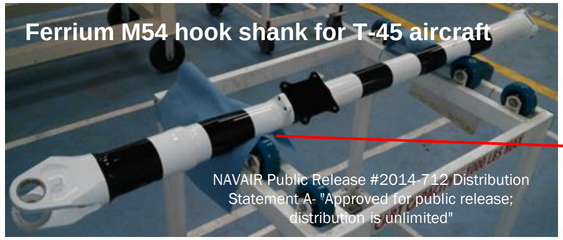
Ferrium S53 roll pin for C-5 aircraft

Space / rocket components

<u>Ferrium M54® structural steel</u>

T-45 hook shank; commercial landing gear evaluations

From materials design to flight in 7 years

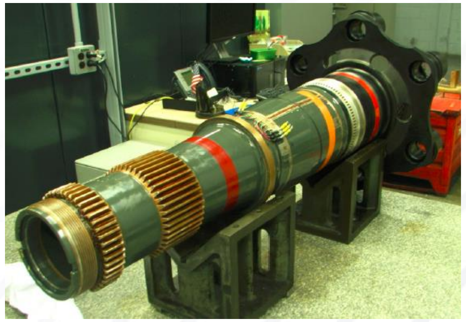


Ferrium M54 hook shank for T-45 aircraft

NAVAIR Public Release #2014-712 Distribution Statement A- "Approved for public release; distribution is unlimited"

<u>Ferrium C64® and C61™ carburizable steel</u>

Qualified by Bell Helicopter, Boeing and Sikorsky for next generation helicopter transmissions for DoD, replacing incumbent steels used for 50 years



Ferrium C61 helicopter rotorshaft for Boeing Chinook, allowing 20% higher power; Production expected to start in 2021

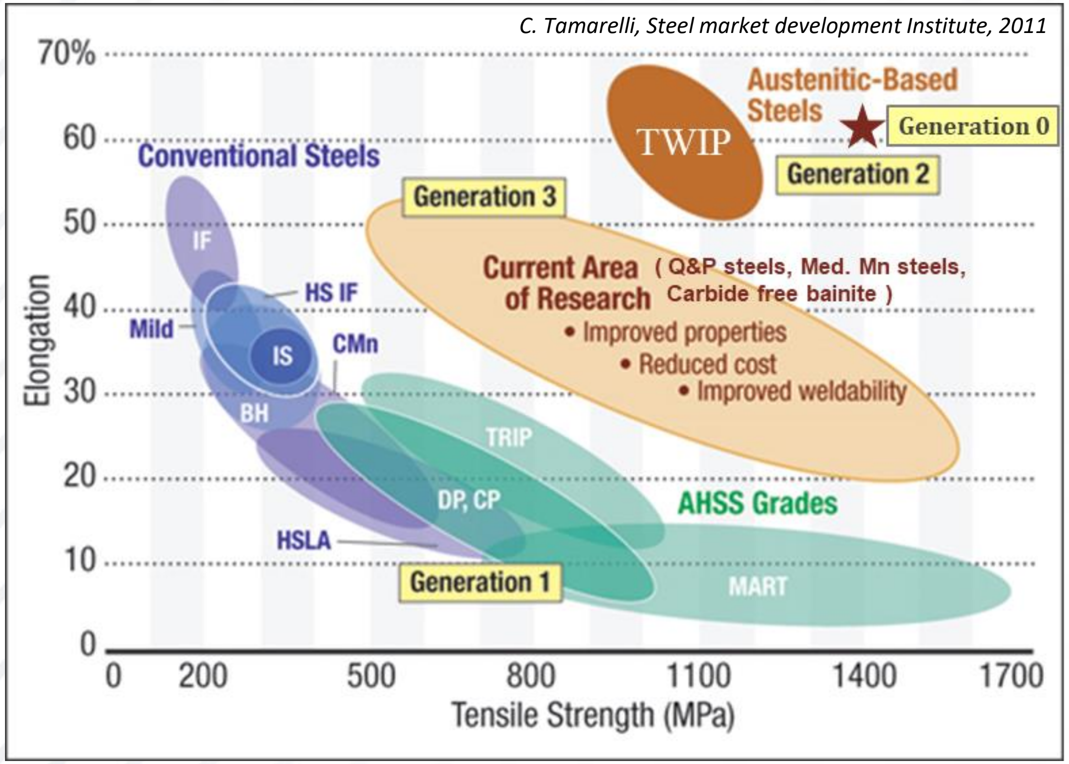
Commercially available from Carpenter Technology

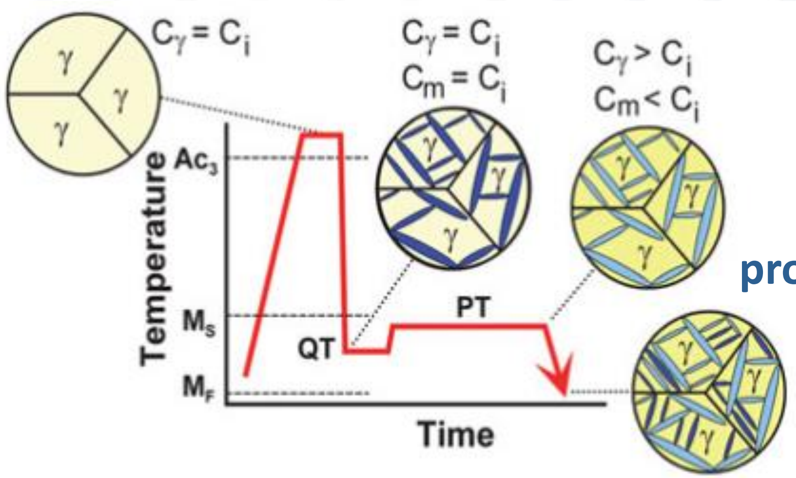
EXAMPLE STEEL PROJECTS AT QUESTEK

- ICME Designed Steel for Energy and Transportation applications

Project	Application	Funding source
High strength, Sulfide Stress Cracking resistant steel	Oil and gas casing and tubulars	Commercial
Weldable, high Cr ferritic steel	Supercritical power generation boiler tubes	DOE funded SBIR program
Low cost, high performance **gear steel**	Automotive transmissions	Commercial
High strength and toughness **castable Ferrium PH48S™ stainless steel**	Structural components	USMC funded SBIR program
Additively as-printed **high strength and toughness steels**	Structural Naval applications	ONR research program
High strength high toughness plate steels	Transport applications	Commercial
Many other Steel development projects related to additive manufacturing…		

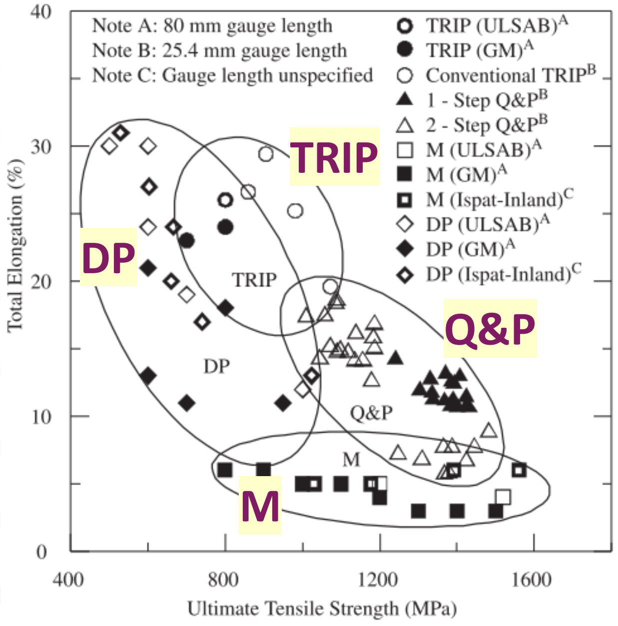
QUENCH AND PARTITION STEELS

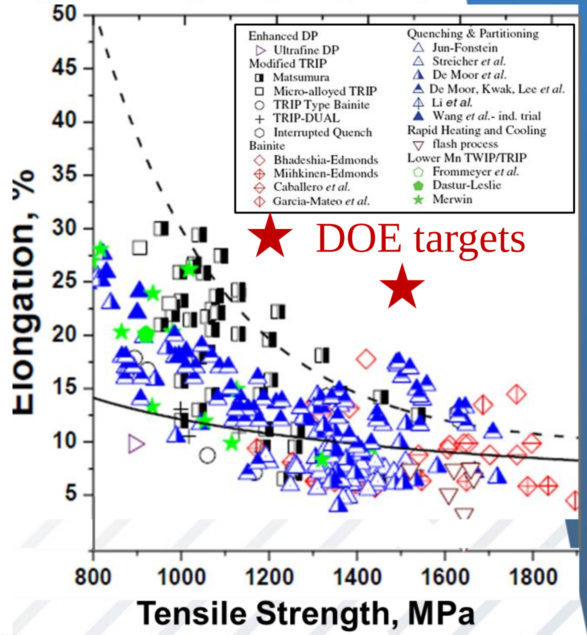




Q&P processing

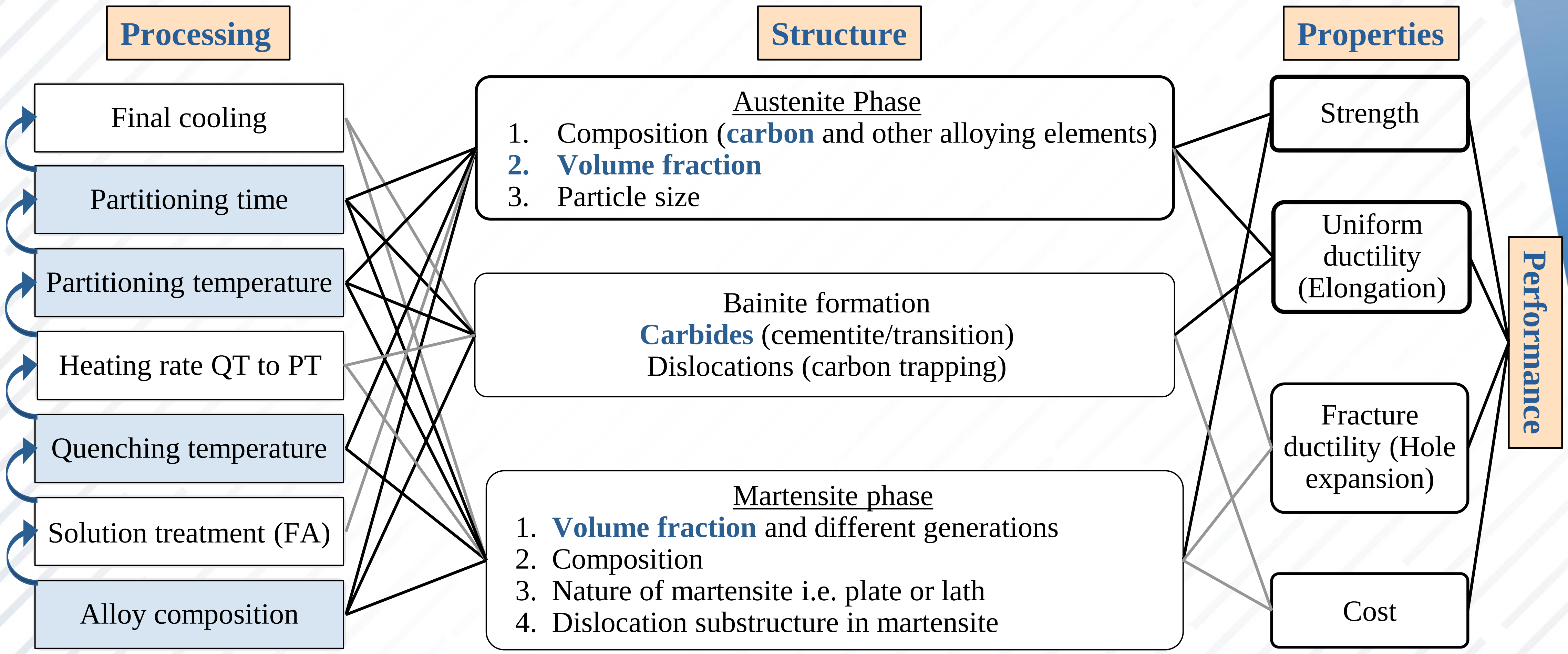
- Mechanical properties of Q&P alloys
  - High strength due to martensite matrix
  - Improved ductility due to TRIP effect of the retained austenite



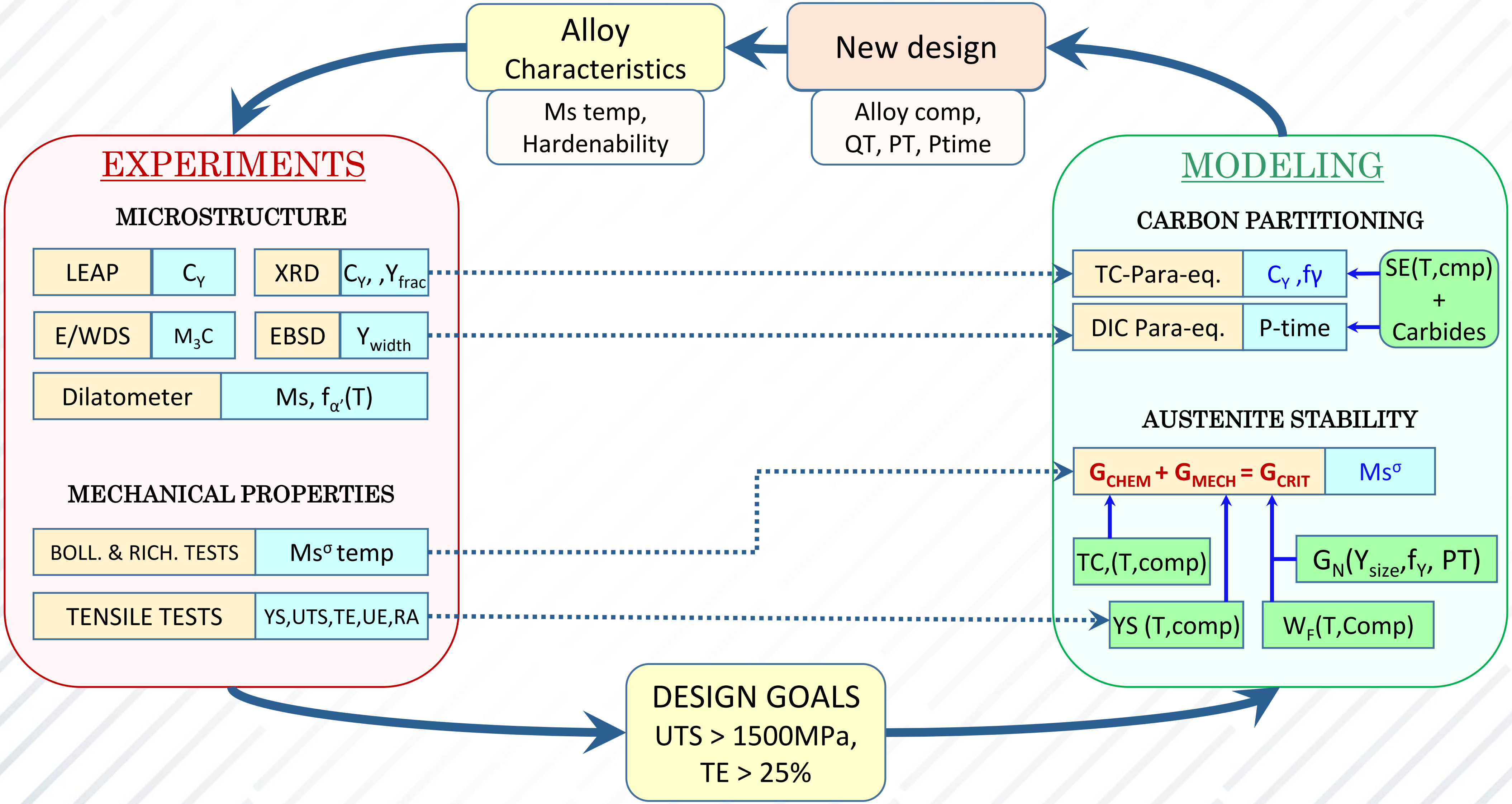


Speer, John G., et al. Materials Research, vol. 8, no. 4, Dec. 2005, pp. 417–23
Matlock, D. K.David K., et al. Jestech, vol. 15, no. 1, 2012, pp. 1–12

MATERIALS SYSTEMS DESIGN CHART



DESIGN FLOWCHART

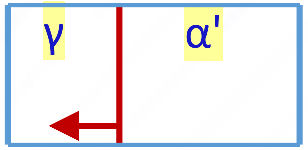


THERMODYNAMIC MODELING

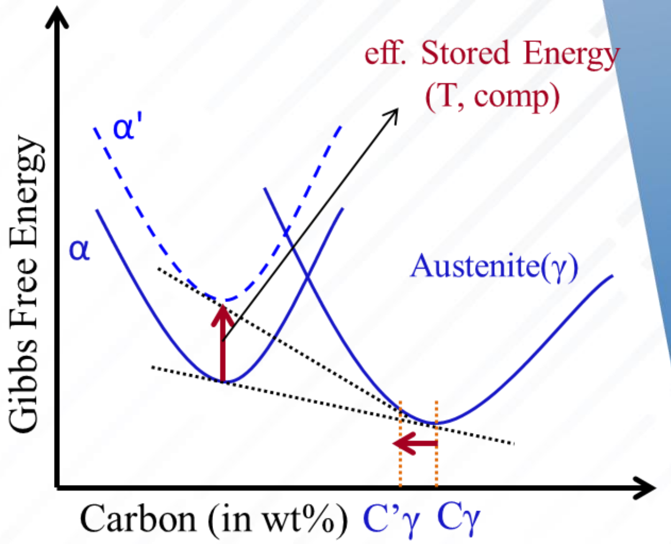
GDIS

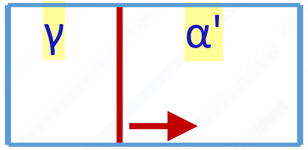
Carbon partitioning model

- Major factors affecting carbon partitioning
  - Alloy composition
  - Partitioning temperature (PT)
  - Quench temperature (QT) – smaller effect
- Para-equilibrium simulations using ThermoCalc© & DICTRA©
  - Chemical potential of carbon same in both phases
  - No movement of substitutional alloying elements
  - Movement of austenite/martensite interface possible
  - added ‘effective stored energy’ contribution to product phase
    - eff. SE = $G_{el} + W_F^{D} + W_F^{SS}$
- Stored energy contribution due to
  - Resistance to interface movement due to **solid solution elements, forest dislocations**

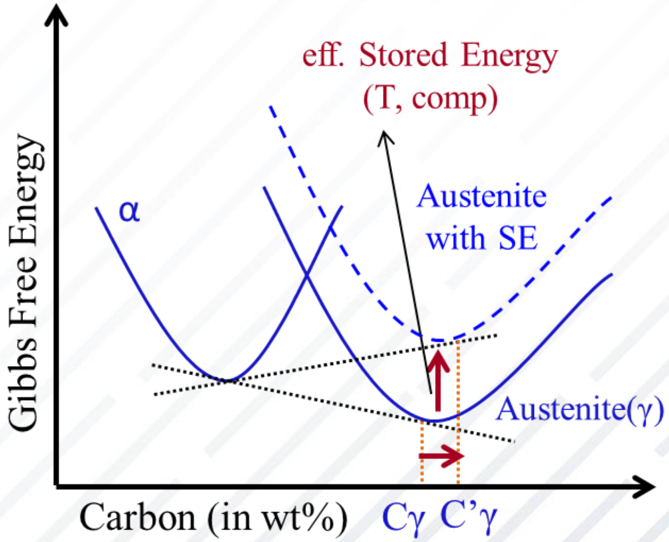


DE added to BCC





DE added to FCC



QT has implemented stored energy models into ThermoCalc PE simulations to predict carbon partitioning

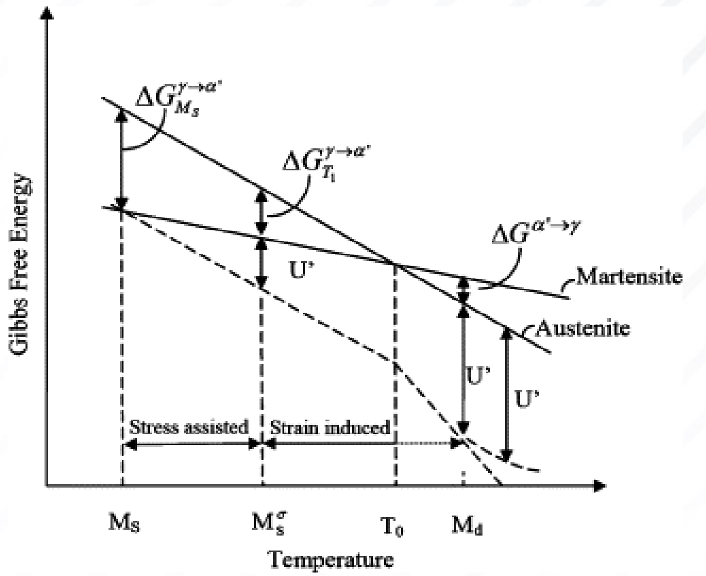
Behera, A. K.; Olson, G. B. , Scr. Mater. 2018, 147, 6–10

THERMODYNAMIC MODELING

GDIS

Retained austenite stability model

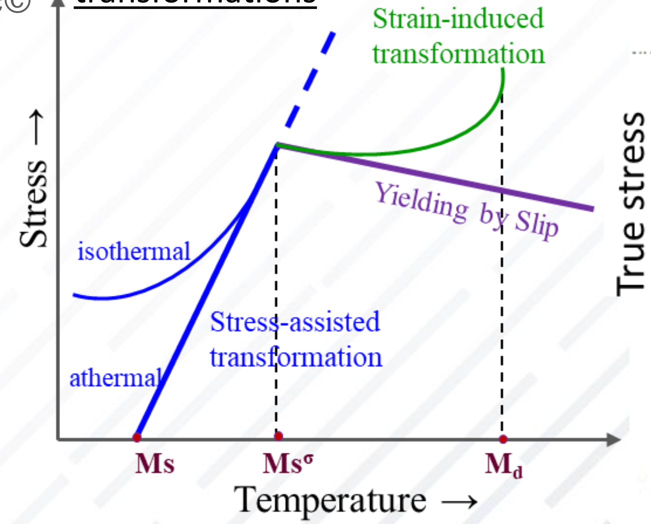
- Major factors affecting austenite stability
  - Chemical composition (esp. carbon content)
  - Morphology / size of retained austenite
- Quantified in terms of the “Ms$^{\sigma}$ temperature”
  - Stress-assisted mode to Strain-induced mode
  - Experimentally measured using uniaxial tensile tests
  - Based on the martensite nucleation theory



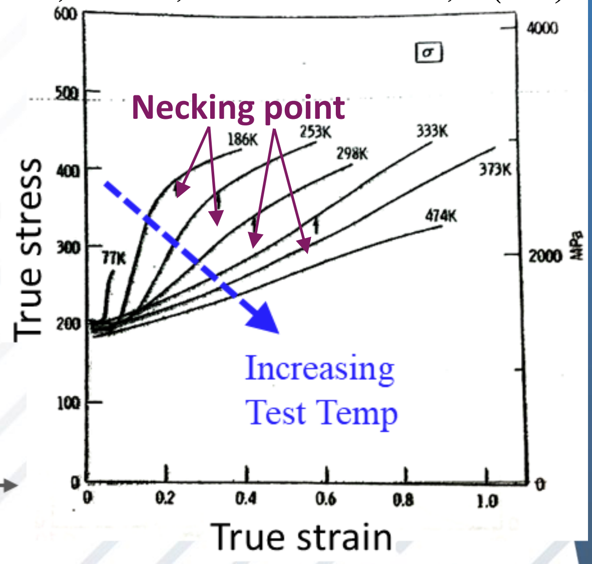
- $\Delta G_{Chem} + \Delta G_{Mech} = \Delta G_{Crit}$ at T=Ms$^{\sigma}$ and σ=YS$_{slip}$
  - $\Delta G_{Chem} = G_{BCC} - G_{FCC} = F(X_i, T)$ - determined using ThermoCalc©
  - $\Delta G_{Mech} = \sigma(\frac{\partial \Delta G_{Mech}}{\partial \sigma}) = -0.718\sigma - 6.85(\frac{\Delta V}{V})\sigma_H + 185.3(1-\exp(-0.003043*\sigma))$
  - $\Delta G_{Crit} = -G_{el} - (\frac{2\gamma}{nd}) - W_F^{D} - W_F^{SS}$

RA stability model utilizing ThermoCalc calculations implemented at QuesTek

Deformation-induced transformations



Olson G.B. , Cohen M., J. Less-Common Metals, 28 (1972)



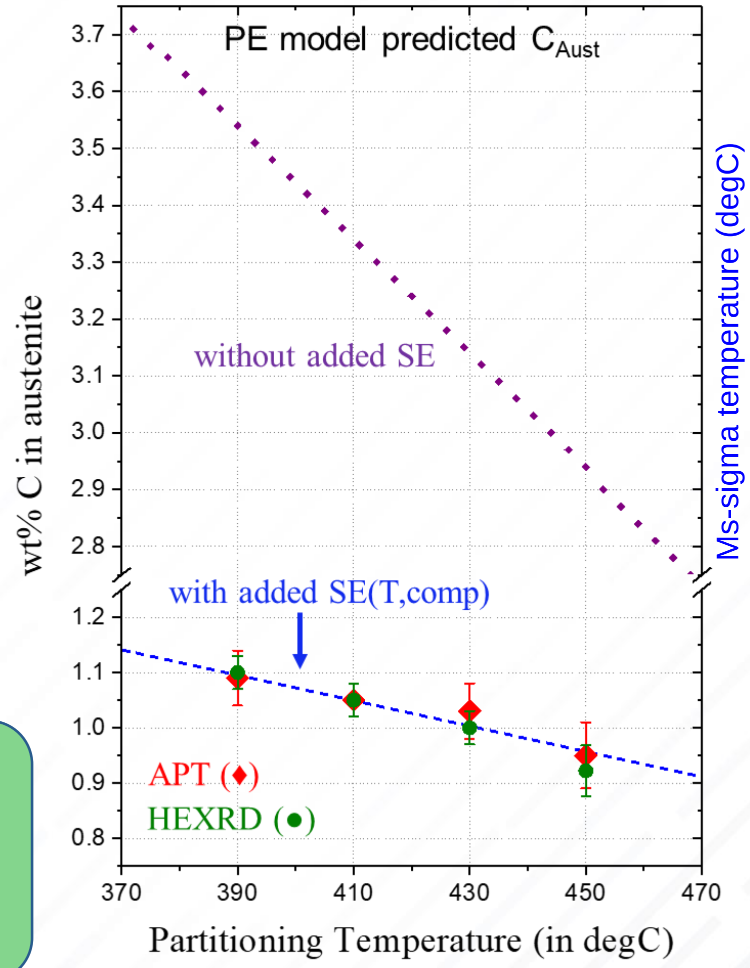
Behera, A.K. & Olson, G.B. JOM (2019) 71: 1375.

ROLE OF PARTITION TEMPERATURE

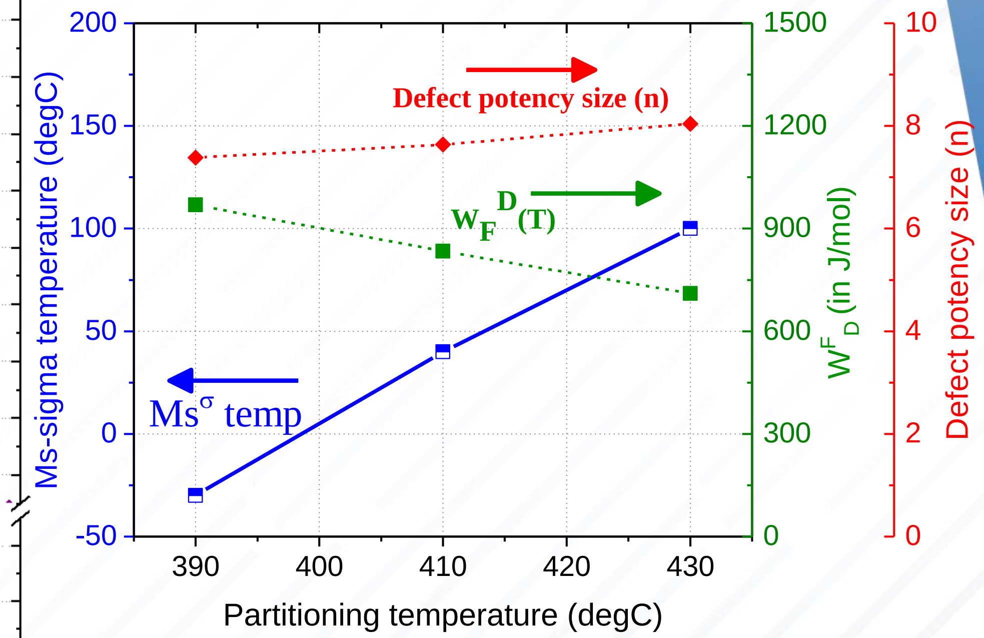
Carbon partitioning model

- 0.2C 2.2Mn 1.5Si 0.2Cr
- Adding eff. SE(T,comp)
  - Reduces the predicted austenite carbon content
  - Reduces its variation with PT as seen in experiments
- $W_F^D = -6.25*PT + 3403$ (in J/mol)

The use of Stored energy model is essential to predict austenite carbon content using ThermoCalc



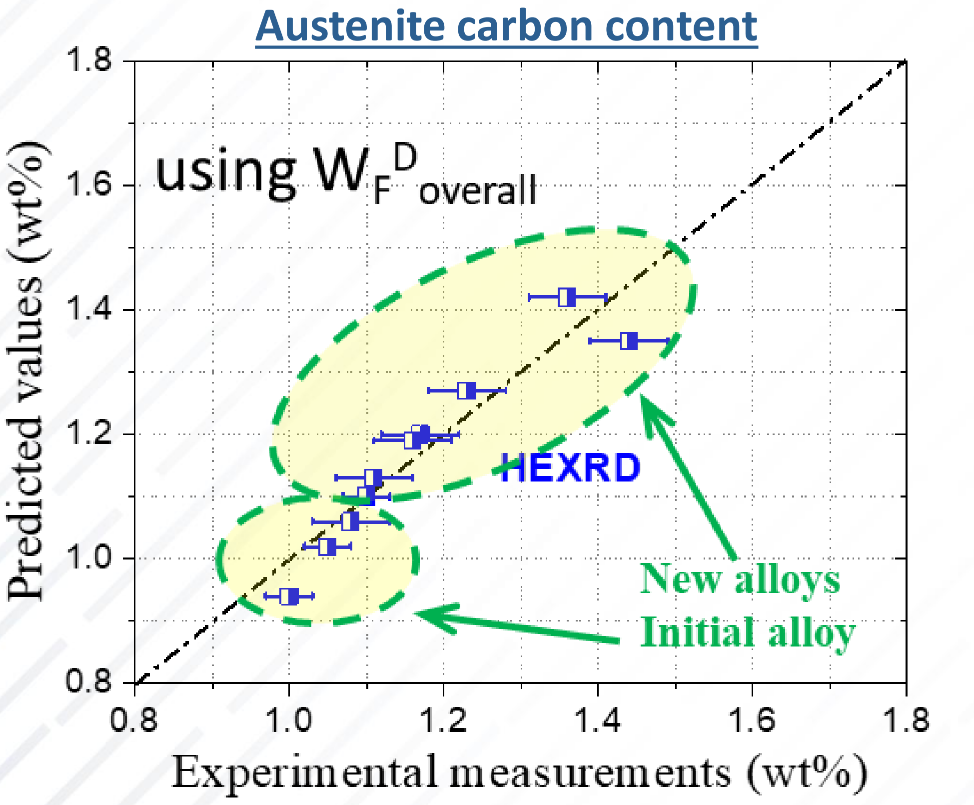
Austenite stability model



- Austenite stability model utilized the W_F^D (T, comp) developed for carbon partitioning model
- The experimentally measured Ms^σ values were used to calibrate the model, specifically the value of defect potency (*n*)

ROLE OF PARTITION TEMPERATURE

- Model validation using a set of **7 new prototype alloy compositions and Q&P processing**
- New designed alloys (composition + QP cycle) showed good agreement of austenite carbon content and austenite stability with predicted values



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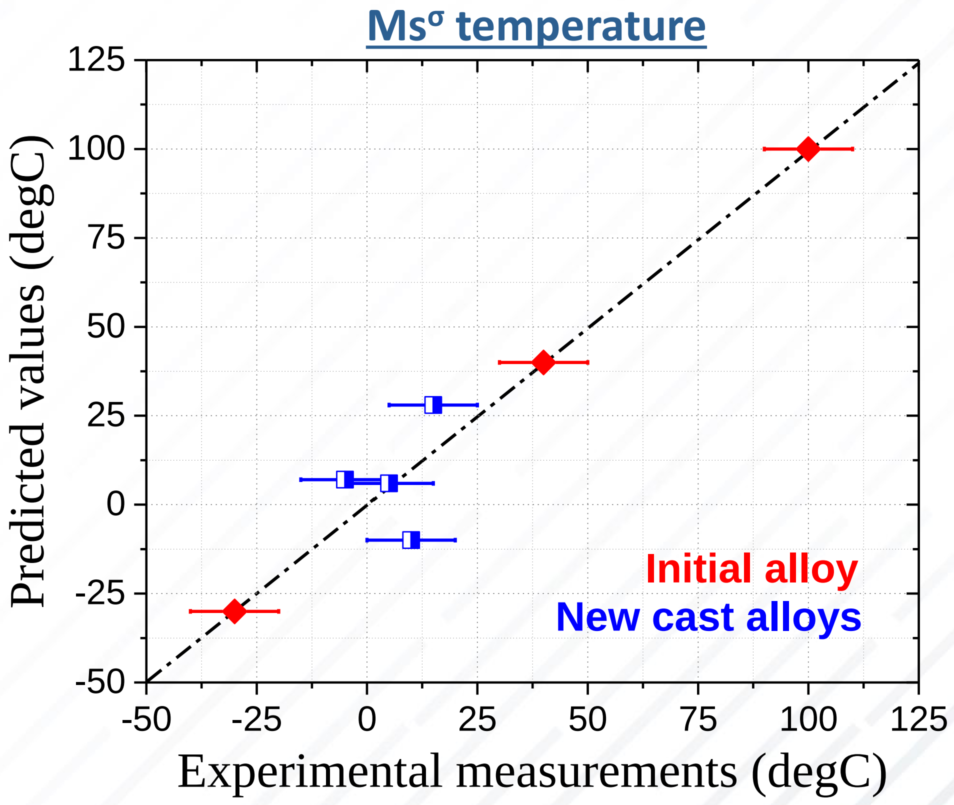


Behera, A.K. & Olson, G.B. JOM (2019) 71: 1375.

Developed models validated and ready to be used for any given alloy + Q&P conditions

Q&P STEEL DESIGN UTILIZING MODELS

Example Q&P processing design:

Alloy composition: Fe-0.18C-2Mn-1.5Si-0.2Mo

Steel	Q&P Cycle	YS, MPa	TS, MPa	TE, %	Ret. γ, %	$C_{austenite}$ at%
Initial	QT=350_2K/s_PT=450°C(100sec)	978	1202	14	10.4	4.7
New Cycle	QT=290_25K/s_PT=420°C(75sec)	1213	1308	16	5.3	5.1

- **ICME-designed Q&P processing cycle showcases improved TS,TE combination**
  - Quench temperature optimized to increase the yield/tensile strength
  - Partition temperature optimized for optimal austenite stability
    - Results in improved elongation due to optimal TRIP effect
  - Improvement in elongation in spite of lower phase fraction (due to carbide precipitation)
  - Further improvement is possible upon limiting the carbide precipitation

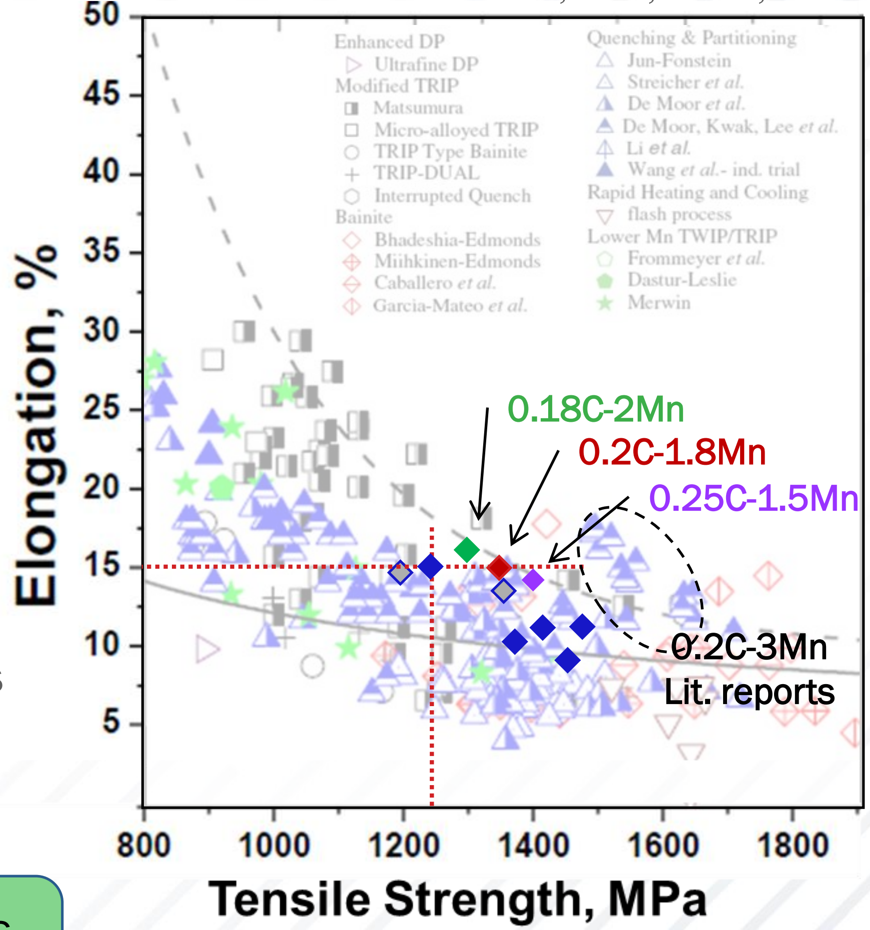
Q&P STEEL DESIGN UTILIZING MODELS

Optimal Q&P process design for different alloys:

Alloy	QT, PT	UTS	UE	TE
0.2C-2.2Mn-1.5Si-0.2Cr	300, 450	1203	-	15
0.2C-2.2Mn-1.5Si-0.2Cr	270, 410	1358	7.7	13
0.18C-2Mn-1.5Si-0.2Mo	290, 420	1308	7.6	16
0.2C-1.8Mn-1.5Si-0.2Mo	310, 420	1342	9.3	14.5
0.25C-1.5Mn-2Si-0.2Mo	275, 410	1471	6.1	11.4
0.25C-1.5Mn-2Si-0.2Mo	335, 430	1406	10.1	14.2

- Optimizing the Q&P processing helped maximize the strength-elongation combination at lower Mn alloying levels
- Further improvement in properties is possible with composition optimization and additional alloying additions

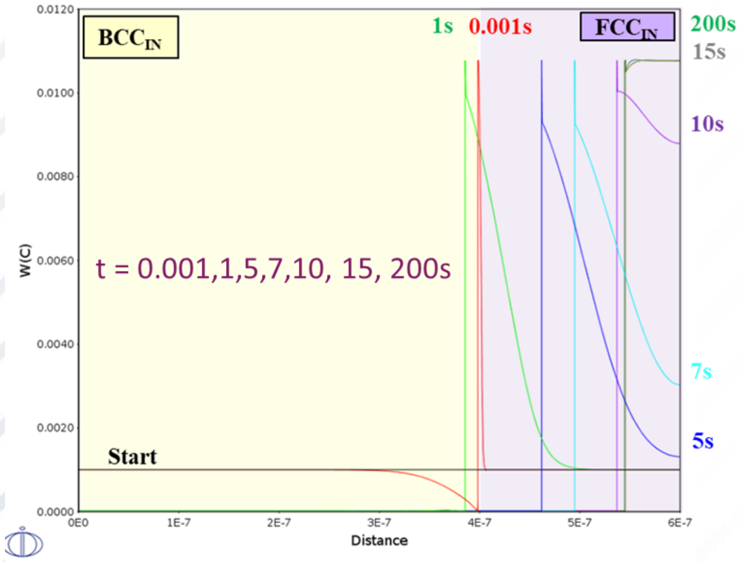
D. K. D. K. Matlock, et. al., Jestech, 2012.

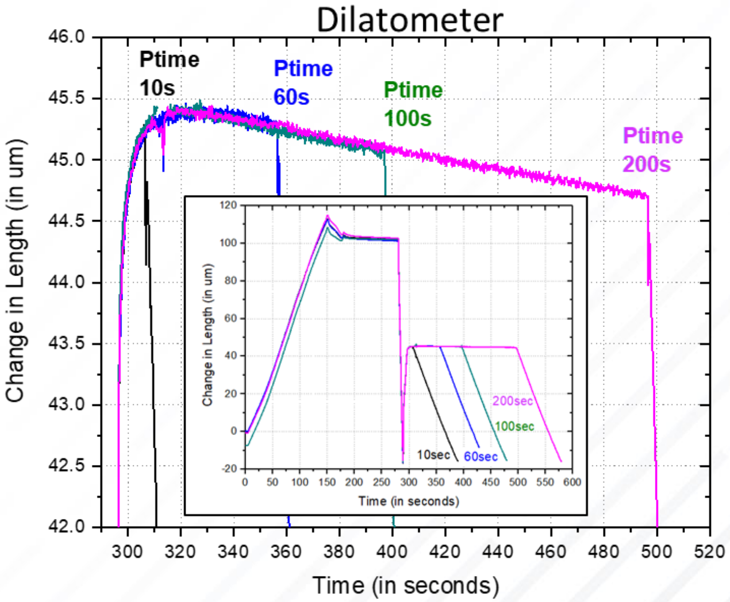


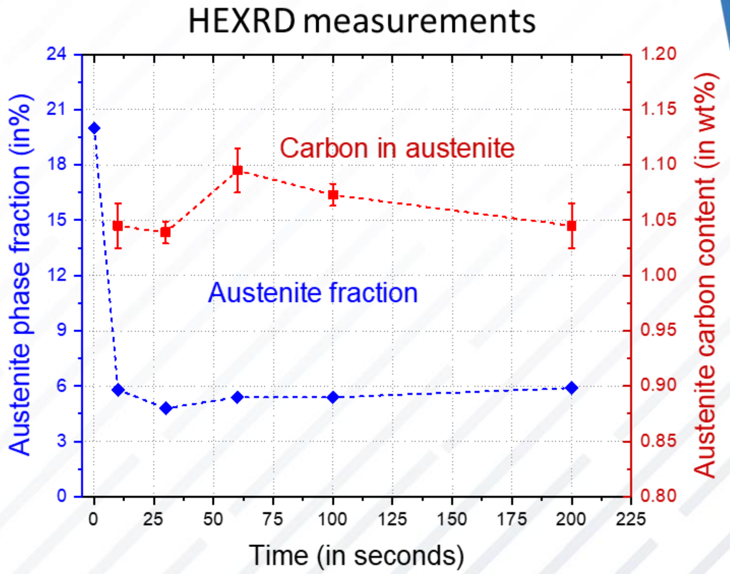
Developed models utilized to design optimal Q&P cycles to achieve properties along the peak performance curve

OTHER ASPECTS OF Q&P INVESTIGATED

- The role of partition time
  - DICTRA© simulations with added effective SE to the BCC phase & modified C in alloy due to carbides
  - Simulations can be used to predict partitioning kinetics for
    - Different steel compositions, different PTs and austenite size
  - Time scale for homogenization matches time for peak change in length from dilatometer







DICTRA calculations with Stored energy model addition can be used to optimize partition time

SUMMARY

- Predictive thermodynamic models were developed and validated for
  - Carbon partitioning during Q&P process
  - Retained austenite stability in the Q&P microstructure
- The role of quench and partition temperature/time on the carbon partitioning and austenite stability were established and quantified
- Design of optimal Q&P process cycles for any composition showcased with use of the developed thermodynamic models
  - Design of optimal composition would take into account weldability, carbide precipitation and other processing challenges
- Further property improvement is currently being investigated via new alloy composition design focusing on
  - Reducing carbide precipitation
  - Increasing the austenite fraction with optimal austenite stability

CURRENT EFFORTS AT QUESTEK

- Currently pursuing industrial partnerships to define
  - The performance metrics for specific application of Q&P steels
  - Exhaustive list of material properties required by end-user
  - The list of material processing constraints/challenges faced by steel producers

- Experimental efforts in internally-funded project towards
  - Optimizing multiple austenite stability for property improvement
    - Influence of retained austenite films vs blocky austenite
  - Development of new Q&P steel grades to ensure
    - Minimal carbide precipitation
      (*utilizing thermodynamic and kinetic models for carbide precipitation*)
    - Adequate spot-weldability

ACKNOWLEDGEMENTS

- ArcelorMittal Global R&D, East Chicago, Indiana
  - Dr. Damon Panahi, Dr. Shrikant Bhat
- Steel Research Group (SRG) at Northwestern University
  - Prof. Gregory Olson

Thank you for your attention!

Any questions?

Contact information:

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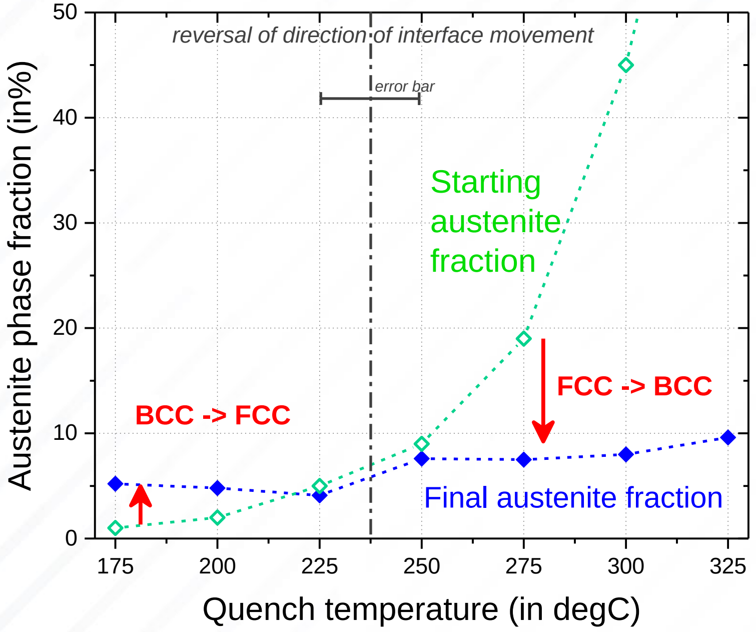
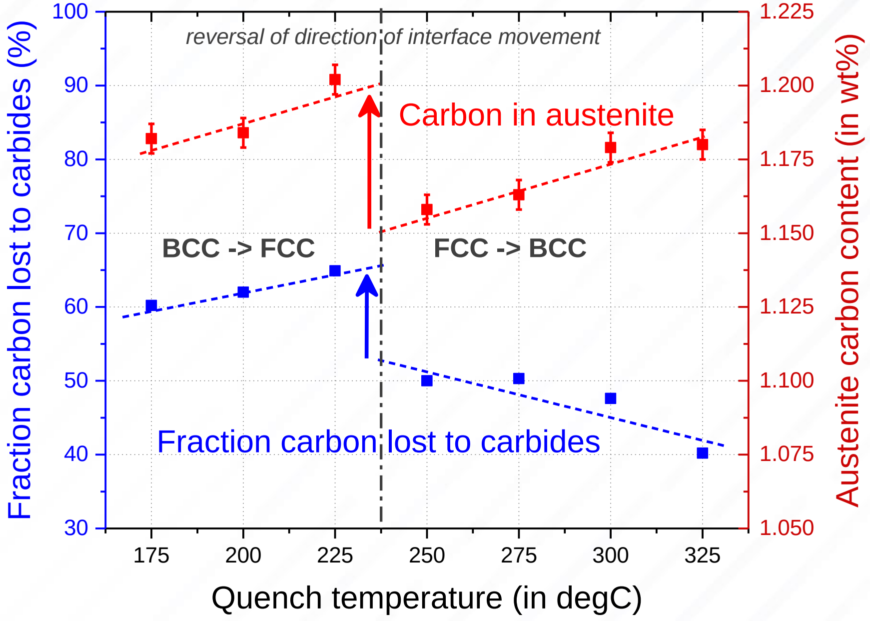
BACKUP SLIDES

ROLE OF QUENCH TEMPERATURE



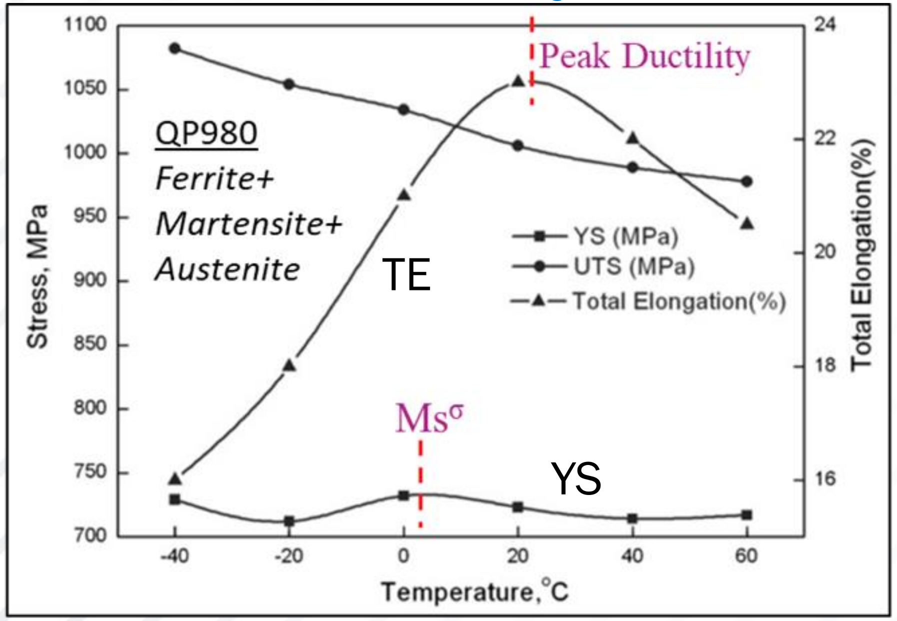


- At higher QT, austenite carbon content decreases with decreasing QT
  - increasing W_F^D due to dislocation density of increasing martensite fraction
- Increase from QT250 to QT225
  - due to reversal of direction of interface motion
- Austenite phase fraction reduces upon reversal of interface motion
- Higher amount of carbide precipitation upon reversal of interface motion
- Sign change of dissipated energy terms upon interface reversal lowers eff. SE

OTHER ASPECTS OF Q&P INVESTIGATED

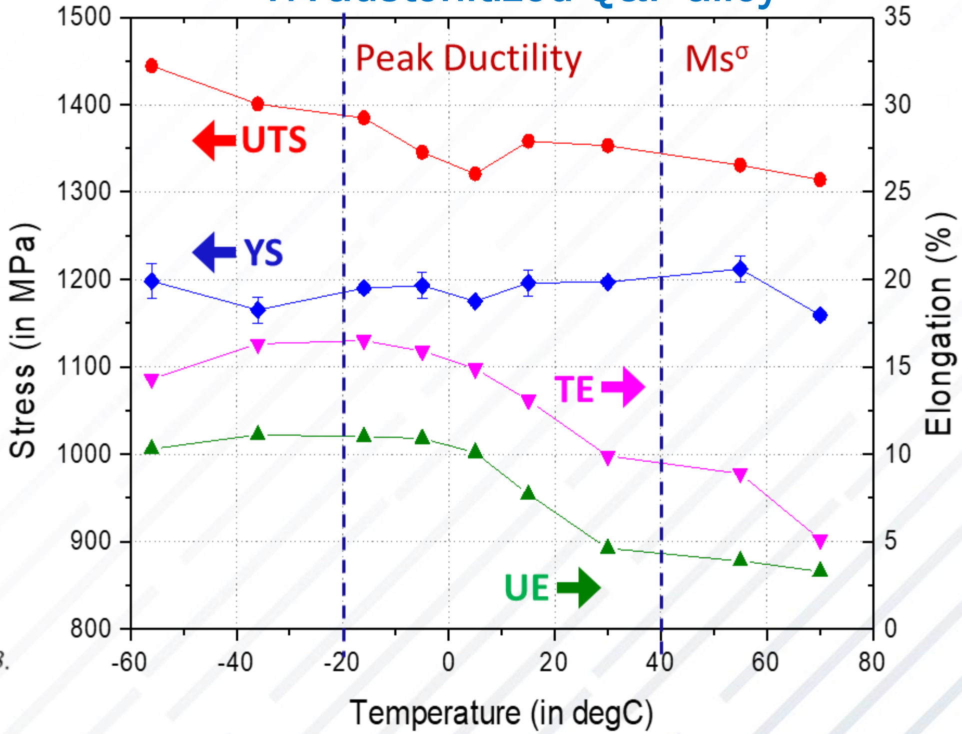
- Multiple Austenite Stability in fully-austenitised Q&P alloys
  - Temperature-dependent ductility variation in the matrix martensite phase
  - Bimodal retained austenite stability due to
    - Inhomogeneous carbon content
    - **Difference in morphology (blocky vs film-type)**

IA austenitized QP980



L. Wang and J. G. Speer, Metallogr. Microstruct. Anal., vol. 2, no. 4, pp. 268–281, Jul. 2013.

FA austenitized Q&P alloy



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