Accelerated Development of Advanced Alloys Via Integrated Computational Materials Engineering

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I.2 USA Materials Genome Initiative

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Dr. Aziz Asphahani
QuesTek Innovations, USA

- ***<u>IWCC Legal Disclaimer:</u>*** **The purpose of this presentation is to guide programs benefiting the copper industry and to provide attendees with information to make independent business decisions**

I.1 Materials Matter

Advanced Materials in Support of Manufacturing / Competitiveness

- **"… materials industry in Japan, especially structural materials, has been the backbone of the whole Japanese industry …"**

  (Cross Ministerial Strategic Innovation Program; Japan, 2016)

- **"… manufacturers must out-innovate their competitors … competitiveness will be defined by the ability to develop and deploy advanced materials …"**

  (white paper/Aerospace Sector; US Council on Competitiveness, 2017)

- **"… recognizing the importance of advanced materials in support of innovations …"**

  (Office of Science and Technology; Washington DC, 2011)

I.2 USA Materials Genome Initiative

(Advanced Materials needed for the US global competitiveness)

Fundamental databases and tools enabling reduction of the 10-20 year materials' creation, along with the "design and deployment" cycle by 50%

National Science and Technology Council (NSTC) / Office of Science and Technology Policy (June 2011)

ICME-Designed *Ferrium*® S53® alloy

Pioneering *Materials by Design®*, as the First "Computationally" designed and qualified alloy to fly (2010)

T-38 Talon landing gear components

Increased strength

Greater ductility

Improved corrosion resistance

Eliminated toxic cadmium-plating

Replaced "Legacy" Alloys

Dragon manned capsule flight test (S53 landing gear components)

II.1 ICME Technologies: QuesTek *Materials by Design®*

QuesTek Scientists & Engineers use thermodynamic and kinetic datasets, along with science-based models, simulation tools and computing power to accurately and quickly design and deploy "Best in Class" materials, by identifying the specific microstructures needed to achieve key properties, essential to enhanced performance.

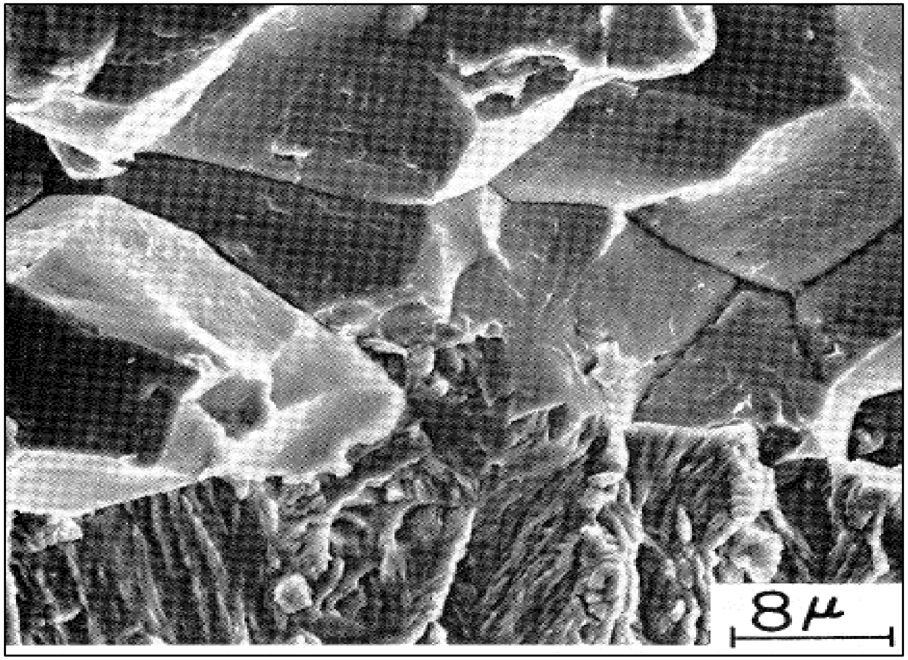
ICME technologies are aimed at improving materials processing and supporting design and deployment of advanced materials (Examples: Fe, Cu, Al, Ti, Ni, Co, Mg, Mo, Nb, W, Ag, …).

Reducing time and cost, along with minimizing risks associated with modified processing, as well as with novel materials design and deployment

(Addressing the priorities set in the USAMaterials Genome Initiative)

Illustration of ICME Design Steps (Advanced Ultra High-Strength Steel)

Failure Mechanism: Intergranular Stress Corrosion Cracking Caused by Hydrogen



Issues:

Stress Corrosion Cracking failures

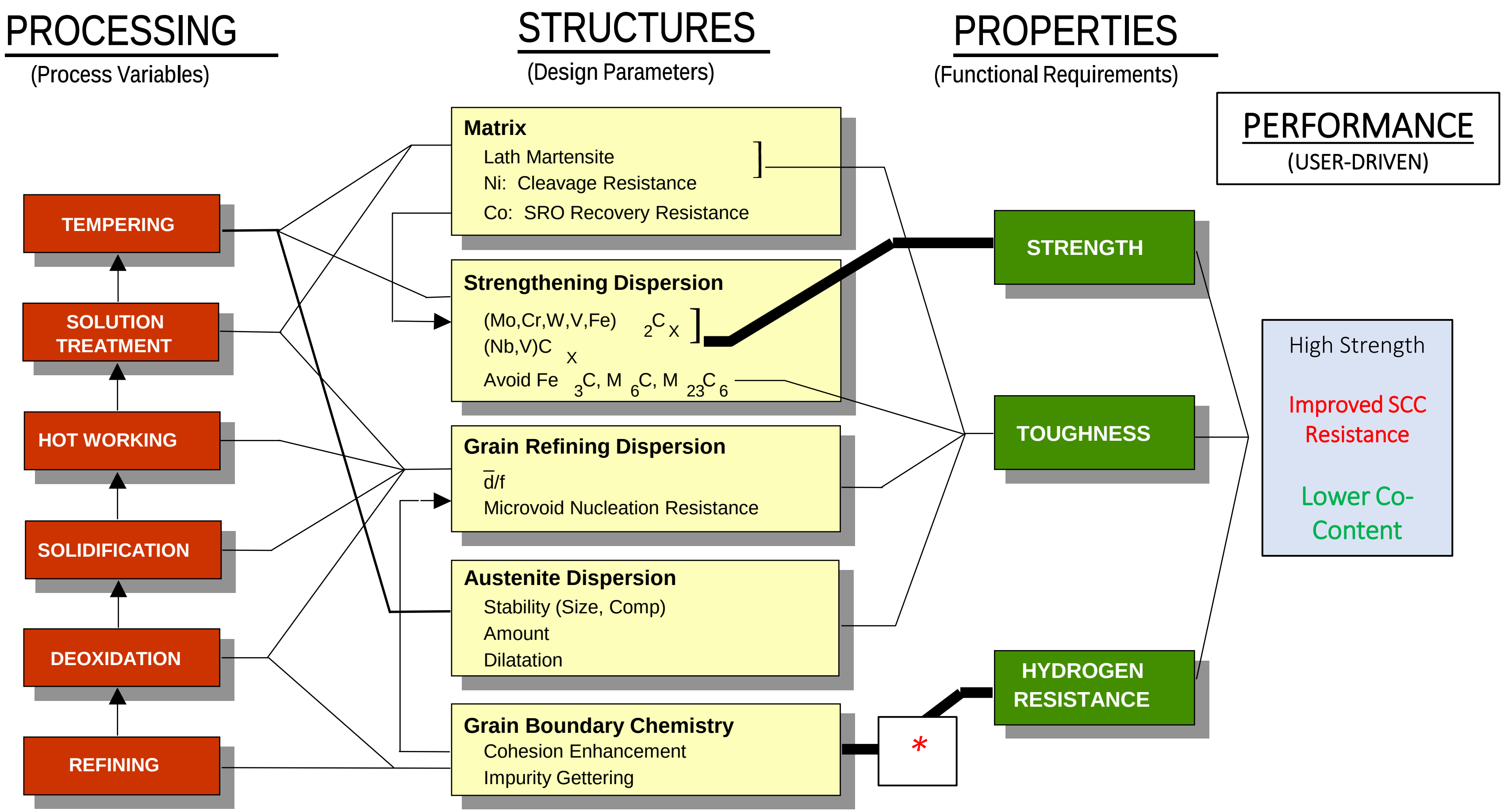
Over $200 million spent annually on military Landing Gears

Issue 1: Susceptibility to Intergranular Stress Corrosion Cracking

Alloy	UTS (Ksi)	K_{IC} (ksi√in)	K_{ISCC} (ksi√in)
300M (1960's)	285	50	15
AMS 6532 13% Co (1980's)	285	115	20

Issue 2: High Cost of Alloying Elements (AMS 6532: 13% Co)

QuesTek ICME Technologies / System-Based Approach (Olson Chart)



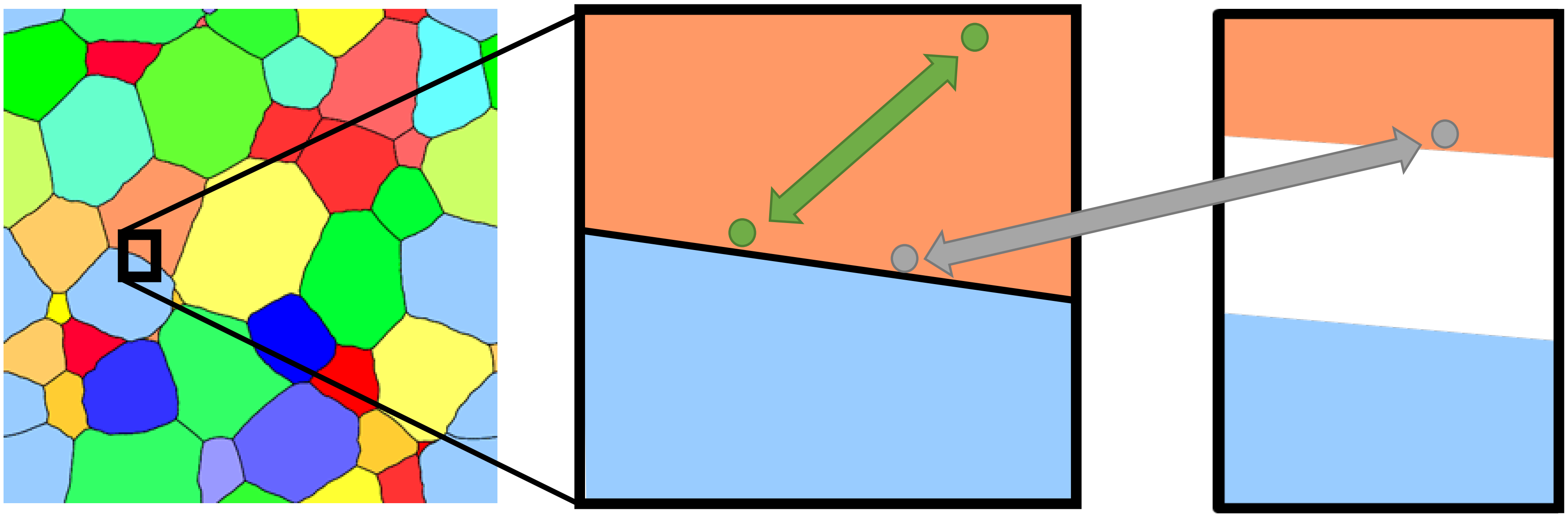
Grain Boundaries Cohesive Energy / Effects of Alloying Elements
(Rice-Wang Model: $\Delta 2\gamma = \sum_i C_i E_i^{pot}$)

Segregation Energy (driving force: Δg_{GB}):

Does solute diffuse to grain boundary from bulk?

Embrittlement potency (E^{pot}):

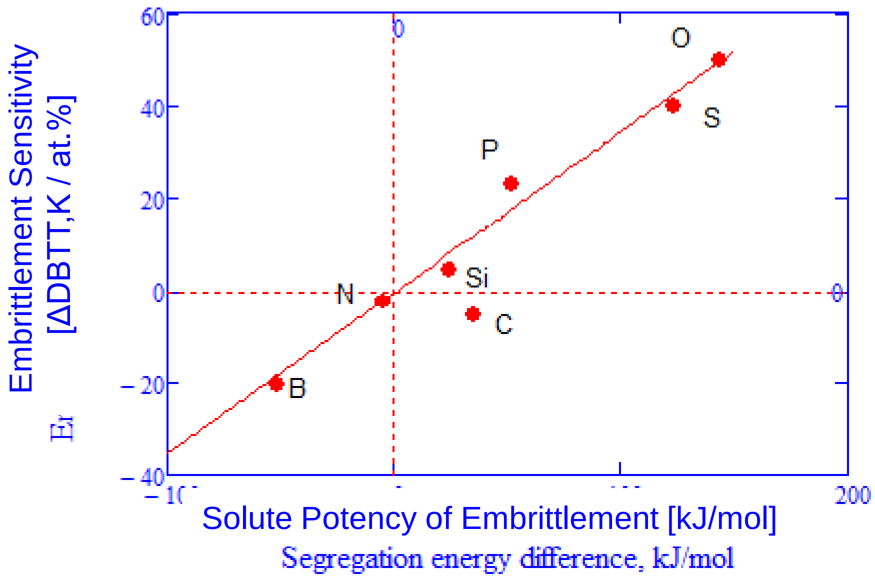
Does solute make it easier to pull apart grains



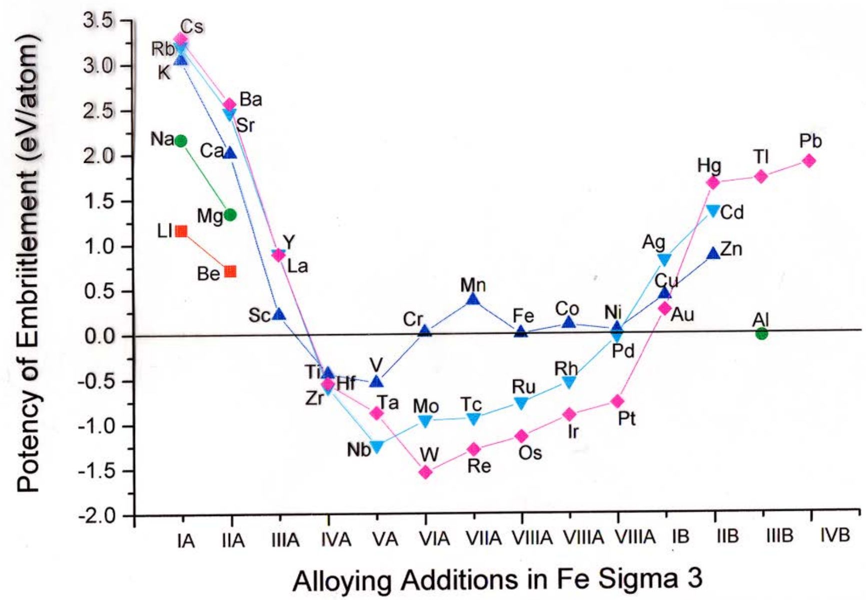
To reduce intergranular brittle fracture: add alloying elements with high propensity to segregate to grain boundaries, along with the potency to improve cohesion

Databases of Embrittling Potency

From Experimental data



Physics-based calculation (DFT)



To reduce brittle fracture: identify the combinations of alloying elements which improve grain boundary cohesion

ICME-Designed *Ferrium®* M54 Ultra-High Strength Steel

Alloy	UTS ksi	K_{IC} ksi√in	K_{ISCC} ksi√in	Grain Boundary Cohesive Energy (Based on $\Delta 2\gamma$ J/m^2)
300M	285	50	**15**	**Lowest**
AMS 6532 **(13% Co)**	285	115	**20**	**Medium**
Ferrium® M54 **(7% Co)**	290	115	**100**	**Highest**

ICME-designed *Ferrium® M54* Hook-shanks (Successful Illustration of USA-MGI)

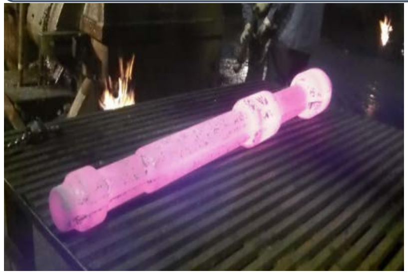
- M54 hook shanks U.S. Navy-qualified with >2.3 x life vs. legacy steel

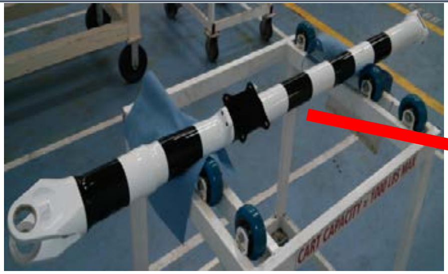
- The U.S. Navy estimates $3 Million saved by deploying M54 steel

M54 approved to replace legacy 300M steel on selected aircrafts for landing gear parts due to greater strength, toughness & SCC resistance

(NAVAIR Public Release #2014-712)

From clean sheet design to qualification and flight in less than 7 years!





QuesTek *Materials by Design®* steel has addressed the priorities set in the Materials Genome Initiative (MGI).

The Ferrium® M54 steel was recognized as an MGI success story (2014)

Materials Innovation Case Study:

QuesTek's Ferrium® M54® Steel for Hook Shank Application

SUMMARY

QuesTek's Ferrium® M54® steel for application in U.S. Navy hook shanks is a notable materials innovation that serves as a current time-to-market baseline for a structure-critical aerospace product. Developed and first commercialized in four years with formal qualification three years later, this innovation was accelerated by the application of computational modeling tools and extensive ferrous materials databases, staff at QuesTek and highly capable companies that they brought to the project, and the strong support of the U.S. Navy throughout the innovation process. Although the non-technical challenges of scheduling small manufacturing runs of new materials and products in commercial production schedules inhibited the overall timeline, this ultimately successful innovation illustrates the strong benefit of implementing the tools that form the core of the Materials Genome Initiative. The following case study explores the specific actions that led to this success in more detail through the development of a "reverse roadmap," which captures and classifies the key activities that accelerated or inhibited the innovation process.

II.2 ICME-designed Copper Alloys

Be-Free Copper Alloys **(Funded by NAVY SBIR / T: N05-009)**

Replace Be-Cu alloys in aerospace applications

Pb-Free Copper Alloys **(Funded by OEM / proprietary applications)**

Replace Highly-Leaded Bronze

NiAl-Bronze for Additive Manufacturing **(Funded by ONR / #N68335)**

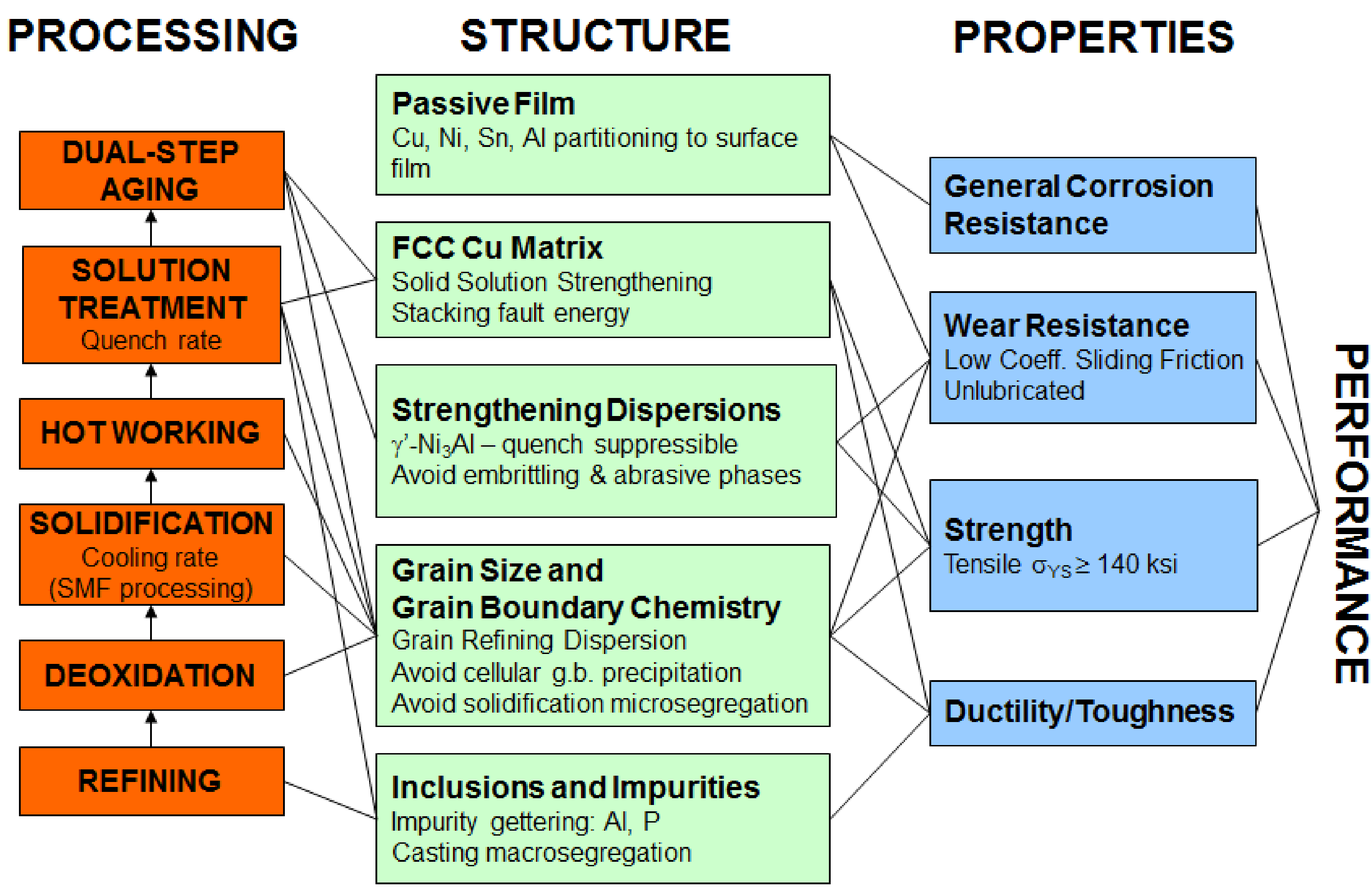
Optimize AM processing & Increase resistance to corrosion/erosion

Be-Free Copper Alloys

- **Need**:
  Eliminate beryllium health concerns through ICME design of a Be-free, high-strength Cu alloy that achieves equivalent strength to Cu-1.9Be alloy
- **Target application**:
  Aerospace bushings
- **QuesTek design concepts**
  - **Precipitation strengthening (Ni_3Al)**
  - **Cellular growth controlled with Sn**
  - **Spray Metal Forming process to avoid low-melting Cu_3Sn**

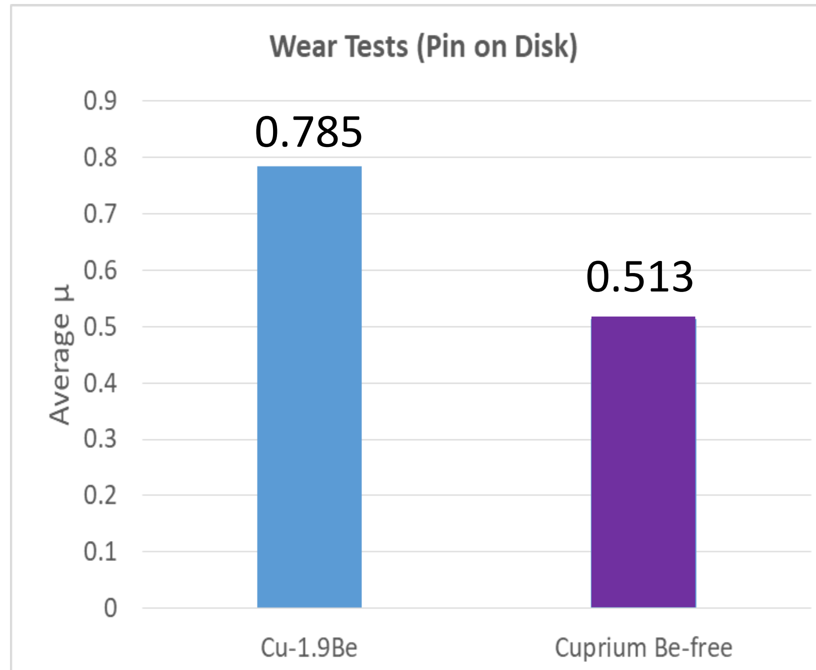
Funded by Navy SBIR (2006-2009)

System-Based Approach (Olson Chart): Be-Free Copper Alloys



Cuprium™ Be-Free high strength Copper alloy

Properties	Cu-Be (Cu-1.9 Be)	QuesTek Cuprium Be-free
0.2 % Yield Strength	140 ksi (min.)	**~140 ksi (typical)**
Elongation	3 - 8%	**~15%**
Strengthening phase (%)	γ' CuBe (~20%)	**γ' Ni_3Al (~20%)**
Wear Ranking	3 (worst)	**2**
Cold workability	Good	**Good-Excellent**
Melting Technique	Various techniques	**Spray metal forming**



ICME-Designed Lead-Free Copper Alloys

- **Need**:
  Replace lead content

- **Target application**:
  Proprietary

- **QuesTek design concepts**

- Alloying with Bi for wear resistance

- Sn addition to increase strength

- Sb and P (to increase miscibility gap width)

Proprietary (Funded by OEM)

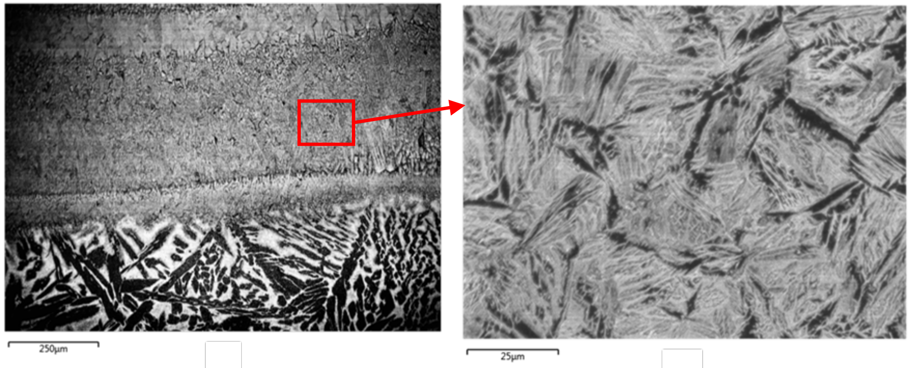
Cuprium™ Pb-Free high strength copper alloy

Property	Cuprium™ Pb-Free	Cu-27-34Pb-2Sn	CDA 93200 (6-8Pb)
0.2 % Y. Strength	15 ksi	13.1 ksi	15 ksi
UTS	21 ksi	20 ksi	35 ksi
Elongation	7%	10.5%	20%
Thermal conductivity @300°F	~0.95 W/(cm K)	~0.95 W/(cm K)	-
Toxicity	No Pb	Contains Pb	Contains Pb

ICME-Designed Novel Nickel Aluminum Bronze (NAB) for Additive Manufacturing

ONR Contract #N68335-17-0318 (Phase I 2017-2018) / Contract #N68335-18-C-0537 (Phase II 2018-2020)

- **NAB products currently utilized in seawater applications are produced through large castings, with long lead times**
- **Additive Manufacturing: to reduce lead time and enhance performance: improved strength, increased corrosion resistance and damping**
- **Goal: ICME design of novel NAB alloys optimized for AM processing**
    - **Produce wire feedstock**
    - **Demonstrate component-level build**
    - **Commercialize technology**



More refined microstructure observed in AM builds vs. castings

QuesTek Activities: Copper Alloys Projects

*** Improved Electrical contact Cu-alloy for high current sliding contact ; NAVY Railgun armature applications**

ONR Funding : N091-069

*** ICME design of "clean" Cu-alloys with high electric conductivity and compatibility with ultra high vacuum**

DOE Funding : addressing trace impurity issues with particle accelerator cavities

*** High-strength, High-electrical and thermal conductivity Cu-alloy for lead frames and connectors**

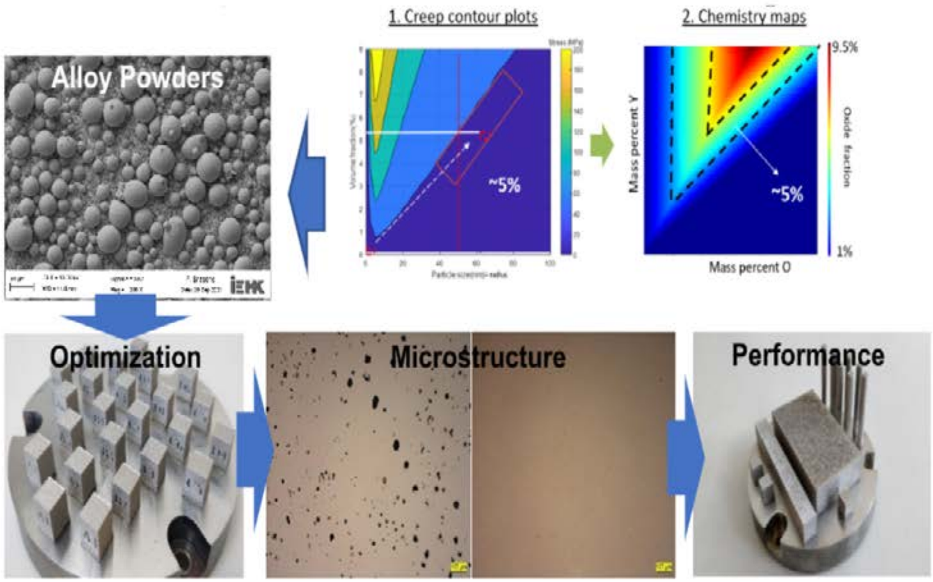
QuesTek Internal Funding : e-Cuprium™ alloy

*** ICME design of "novel" Cu-alloy with improved electric conductivity and resistance to corrosion/oxidation**

Proprietary : addressing environmental issues with Tin coatings

Modeling/Simulation of ODS materials processing routes for Additive manufacturing (EU *topAM* program, *4yrs. / €6MM*)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 958192.



modelling of creep contour plots and chemistry maps; **top left:** powder of AM100; **bottom left**: AM process optimization; **bottom center**: density analysis; **bottom right**: production of specimens for mechanical and corrosion testing.

RWTH AACHEN UNIVERSITY · DECHEMA Forschungsinstitut · Hochschule Osnabrück · KME · INDUTHERM · Linde · QuesTek Europe AB · RISE · Universidad Complutense Madrid · KANTHAL · Sieć Badawcza Łukasiewicz · VDM Metals · La Rochelle Université · Zoz Group · Institute of Physics of Materials

Gas burner head
Honeywell Kromschröder

Engineering Concurrency (Combining alloy, process and product design)

- **Novel oxide dispersion strengthened (ODS) Fe, Ni & Monel/NiCu alloys**
- **ICME-designed and optimized for additive manufacturing**
- **Gas burner heads and hi-temp Heat exchangers**

III- Accelerated Insertion of Materials (AIM) Methodologies
III.1 Qualification of AM-Built Parts (DARPA Ni-base Superalloy 718+)

Process modeling / microstructural-based prediction of properties

Mechanistic Models Microstructure-base insights → Calibrated to data (from 2 lots of powder) → AIM Predicted Properties

$$\sigma_{yield} = \sigma_{yield}\left(D_{gr};\, f_{\gamma};\, f_{\gamma'_p};\, f_{\delta};\, f_{\gamma'_s};\, r;\, \gamma_{APB}\right)$$

$$= f_{\gamma+\gamma'_s}\sigma_{\gamma+\gamma'_s} + f_{\gamma_p'}\sigma_{\gamma_p'} + f_{\delta}\sigma_{\delta}$$

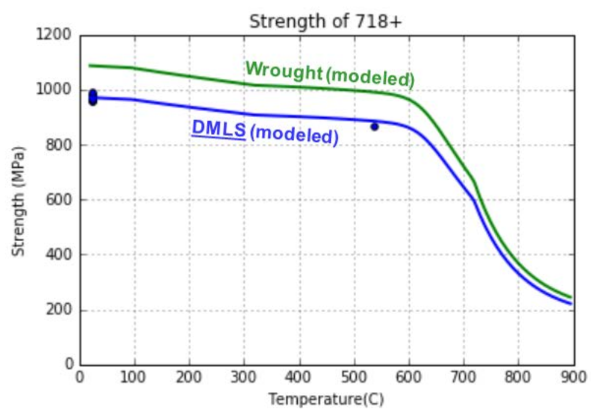
$$\sigma^{\gamma'_p} = \sigma_0^{Ni_3Al} + \Delta\sigma^{SS}(C_i)$$

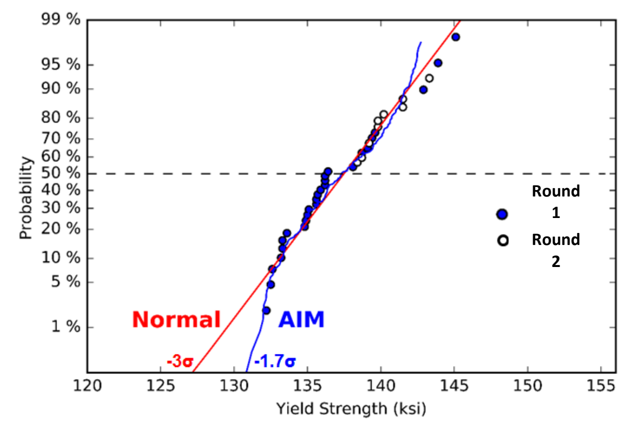
Strengthening in primary γ' due to base strength of Ni_3Al and solid solution strengthening

Strength of δ phase extracted from YS of soln. treated material

$$\sigma^{(\gamma+\gamma'_s)} = \sigma^{HP}(D_{gr}) + \sigma^{SS}(C_i) + \sigma^{Precip}\left(f_{\gamma'_s};\, r;\, \gamma_{APB}\right)$$

Strengthening in γ matrix includes grain size, solid solution and secondary γ' precipitate strengthening





III.2 *Materials Concurrency*™ in support of Engineering Concurrency (Concurrency of Additive Manufacturing and Innovative Design)

Re-design Systems

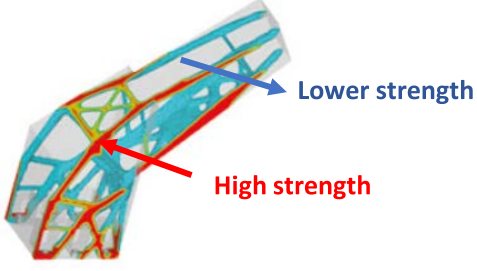
20 pieces sheet metal | One piece AM Part

CT Advanced Manufacturing Co.

Re-engineer Materials

Process Parameters Location-specific ($\sigma_{Resid.}$, Temp, Time)

Microstructure evolution property predictions at key locations



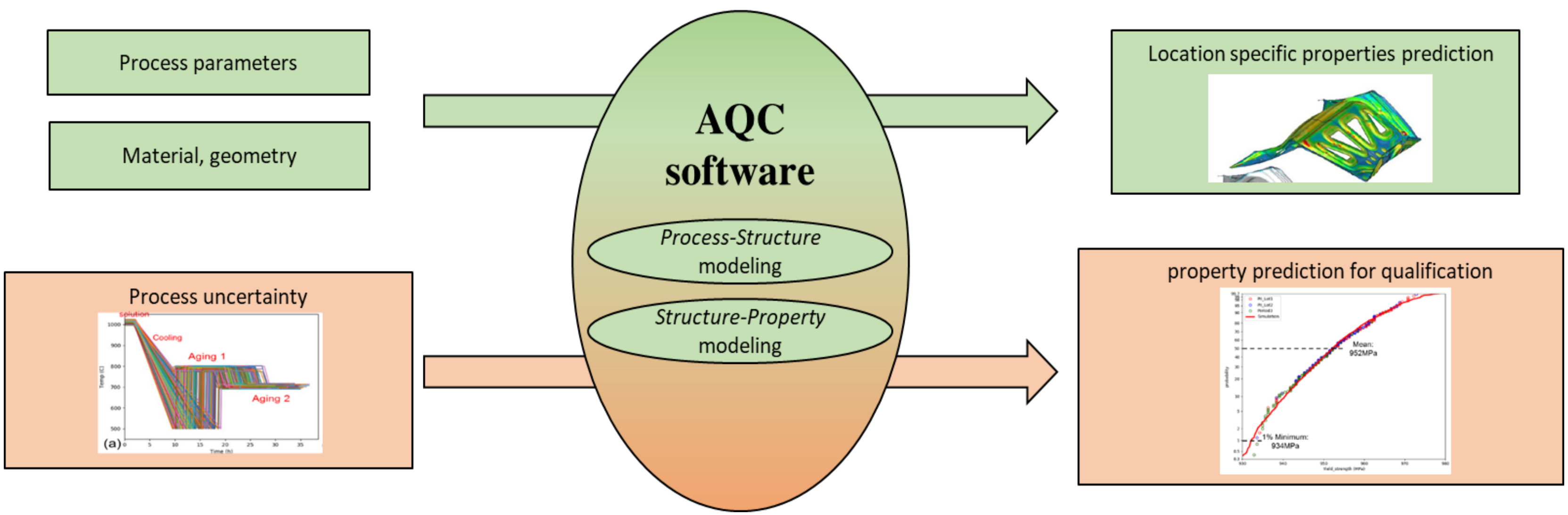
Digital Alloys Co

Issues: Process Reproducibility, inconsistent properties and Performance Reliability of AM-built parts

Need: Accelerate qualification and certification of AM-built parts, via informed simulations

QuesTek experience with Accelerated Insertion of Materials (AIM) methodologies and its expertise in Integrated Computational Materials Engineering (ICME) technologies are being focused on addressing the industry goal with materials science-based predictive software

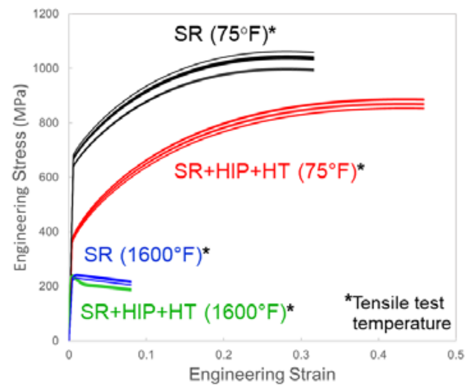
QuesTek AQC "Predictive Software" linking: Process-Microstructure-Property-Performance



Award-winning Predictive Technology for AM-Built Parts
(QuesTek AQC Software)

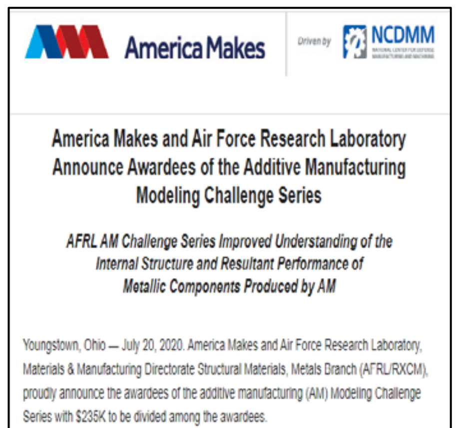
- **QuesTek AQC (Accelerated Qualification and Certification) software is built on Materials Science captive knowledge and Physics-based models.**
- **The AQC success in predicting properties of Additively Manufactured parts, is being extended to other manufacturing processes.**

AFRL: AM accurate models for trusted predictions



Robust Scientific Models: Accurately predict property of IN 625 AM parts (varying heat-treatment, orientations and surface finish)

Limited input Data: only 4 calibration data points used



America Makes | Driven by NCDMM

America Makes and Air Force Research Laboratory Announce Awardees of the Additive Manufacturing Modeling Challenge Series

AFRL AM Challenge Series Improved Understanding of the Internal Structure and Resultant Performance of Metallic Components Produced by AM

Youngstown, Ohio — July 20, 2020. America Makes and Air Force Research Laboratory, Materials & Manufacturing Directorate Structural Materials, Metals Branch (AFRL/RXCM), proudly announce the awardees of the additive manufacturing (AM) Modeling Challenge Series with $235K to be divided among the awardees.

Materials Concurrency™ in support of Engineering Concurrency
A Business Reality

Jony Ive (Apple Chief Design Officer)
New York Times, June 16, 2014

"... Deep in the culture of Apple is this sense and understanding of Design, Developing and making.

... Form, Materials and Process are beautifully intertwined-completely connected ..."

Anodizable Aluminum

60% stronger than standard aluminum

(19) **United States**
(12) **Patent Application Publication** (10) **Pub. No.: US 2015/0090373 A1**
Gable et al. (43) **Pub. Date: Apr. 2, 2015**

(54) **ALUMINUM ALLOYS WITH HIGH STRENGTH AND COSMETIC APPEAL**

(71) Applicant: **Apple Inc.**, Cupertino, CA (US)

(72) Inventors: **Brian M. Gable**, Santa Clara, CA (US); **James A. Wright**, Los Gatos, CA (US); **Charles J. Kuehmann**, Los Gatos, CA (US); **Brian Demers**, San Jose, CA (US); **Chune-Ching Young**, Taoyuan County (TW); **Chun-Hsien Chiang**, Tainan (TW)

(21) Appl. No.: **14/502,943**

(22) Filed: **Sep. 30, 2014**

Related U.S. Application Data

(60) Provisional application No. 61/884,860, filed on Sep. 30, 2013, provisional application No. 62/047,600, filed on Sep. 8, 2014.

Publication Classification

(51) **Int. Cl.**
C22F 1/053 (2006.01)
C22C 21/10 (2006.01)

(52) **U.S. Cl.**
CPC *C22F 1/053* (2013.01); *C22C 21/10* (2013.01)
USPC **148/549**; 148/439

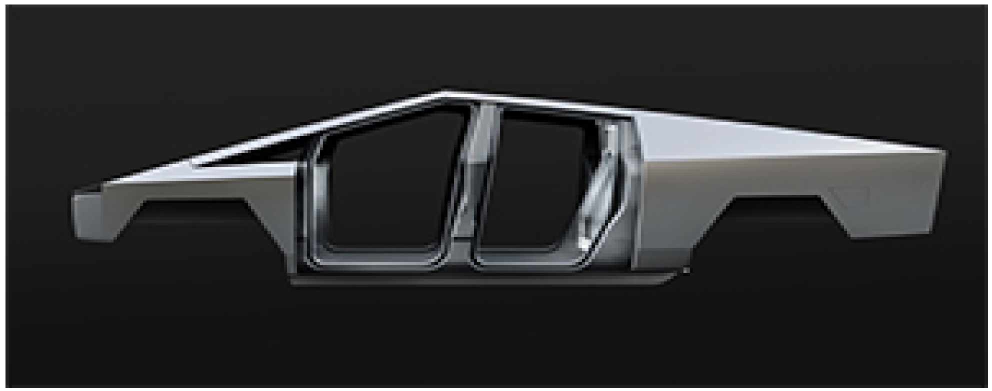
(57) **ABSTRACT**

The disclosure provides an aluminum alloy including having varying ranges of alloying elements. In various aspects, the alloy has a wt % ratio of Zn to Mg ranging from 4:1 to 7:1. The disclosure further includes methods for producing an aluminum alloy and articles comprising the aluminum alloy.

J. Wright, Ph.D. (Northwestern, Olson), 2002; QuesTek 2002-2012
C. Kuehmann, Ph.D. (Northwestern, Olson), 1994; QuesTek 1996-2012
C.-C. Young, Ph.D. (MIT, Olson), 1988

Engineering Concurrency:
Combining *Materials Concurrency™* with Innovative Design

Tesla creates new team to accelerate use of new materials in its products



- **Tesla's Dr. Keuhmann created a new cross-company material engineering team to develop new, advanced materials**

***The idea is to accelerate the adoption of new materials and processes – helping to bridge the gap between materials science and part design"* David Nelson**

https://electrek.co/2021/04/22/tesla-creates-new-team-accelerate-use-materials-products/

Concurrency of Design / Innovative Materials

Elon Musk ✓
@elonmusk

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Replying to @Robotbeat @Jon128123 and 8 others

SpaceX metallurgy team developed SX500 superalloy for 12000 psi, hot oxygen-rich gas. It was hard. Almost any metal turns into a flare in those conditions.

7:40 PM - 22 Dec 2018

IV- Materials Informatics Outlook

(Predictive Capabilities for Novel / Advanced Materials)

Big Data
High-throughput
(Experimental; Calculated DFT)

Uncertainty Quantification

Genomic data / CALPHAD
Validated Thermodynamic/Kinetic data
(Science-based)

Machine Learning
(Multiple descriptors simulations)

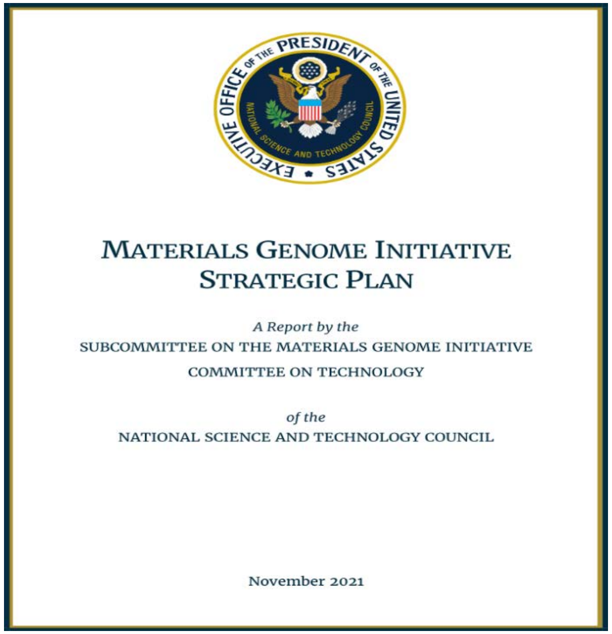
ICME
(Physics-based models)

Artificial Intelligence
Discover Novel compounds "of interest"
(no specific insight required)

***Materials by Design®* (AIM)**
Deploy "engineered" advanced materials
(Atomic and Microstructure insight)

IV.1 Materials Innovation Infrastructure

(USA National Science & Technology Council, November 2021)

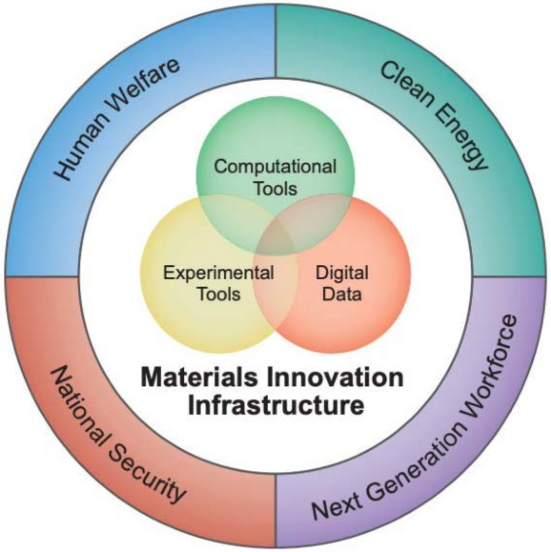


MATERIALS GENOME INITIATIVE STRATEGIC PLAN

A Report by the
SUBCOMMITTEE ON THE MATERIALS GENOME INITIATIVE
COMMITTEE ON TECHNOLOGY

of the
NATIONAL SCIENCE AND TECHNOLOGY COUNCIL

November 2021



Materials Innovation Infrastructure
Integrated Materials Platforms

"… the Materials Genome Initiative works to expand integrated capabilities ... Many research centers provide substantial data infrastructure.

… However, Integrated Materials Platforms are required to breakdown barriers between materials discovery and deployment.

… These materials platforms would serve as innovation nodes of the Materials Innovation Infrastructure …"

(USA National Science & Technology Council ; November 2021)

Materials Innovation Infrastructure

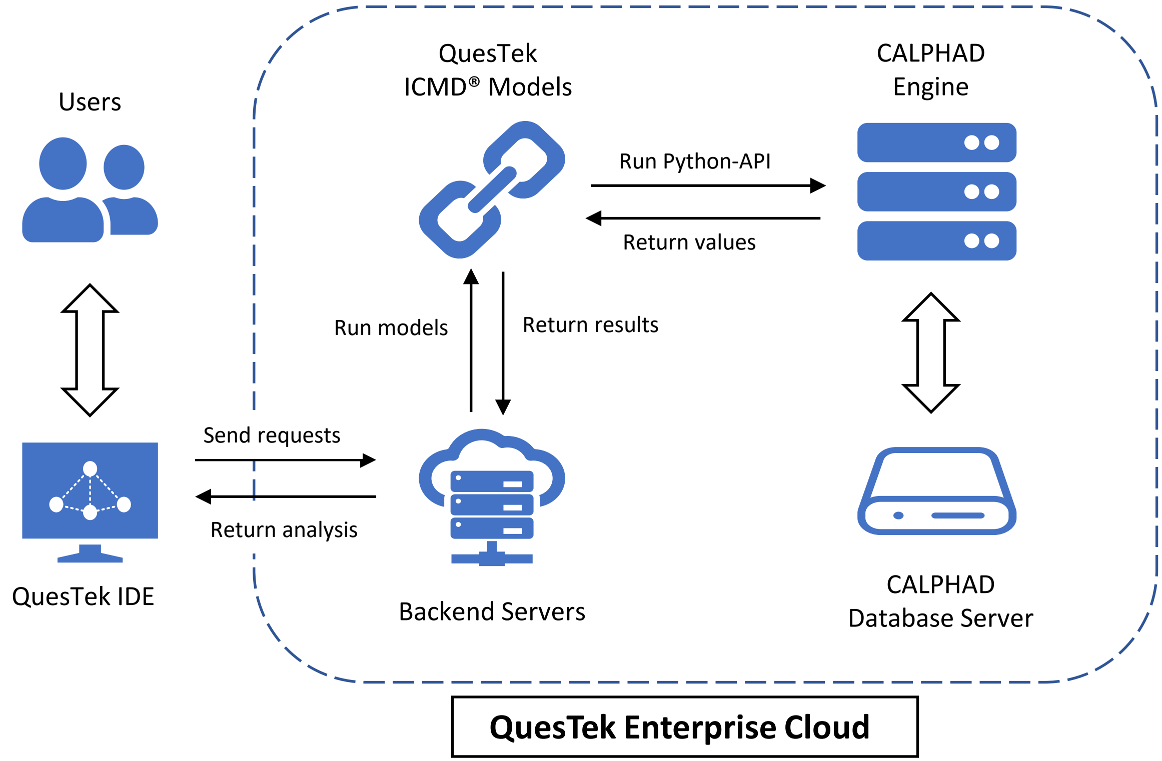
QuesTek Integrated Computational Materials Design and Deployment

QT /ICMD® Platform

Category	Name	Application
Materials Design	**Alloy Design Toolkit**	Major alloys design
	Coating Design Toolkit	Design of material coatings/interfaces
	Gradient Design Toolkit	Design functionally graded materials by additive manufacturing
Materials Qualification	**Accelerated Q&C Toolkit**	Major alloys qualification (focus on additive manufacturing)
Materials Informatics	**Additive Informatics Toolkit**	Analysis tools and datasets for additive manufacturing information
	Corrosion Informatics Toolkit	Analysis tools and datasets for corrosion, CMAS, aqueous dynamics information
	Functional Thermoelectric Toolkit	Analysis tools and datasets for thermoelectric dynamics information
	Microscopy Informatics Toolkit	Analysis tools for microscopy data/images with Machine Learning
Materials Simulation	**CALPHAD Simulation Toolkit**	Running CALPHAD calculations/simulations
	Numerical Simulation Toolkit	Running numerical (MOOSE, ABAQUS, SYSWELD, PRISMs, Nalu etc.) simulations
QT / ICMD® Integrated Design Engine (IDE)	**IDE Infrastructure**	Core IDE front-end / back-end functionality
	IDE Workspace Implementation	Internal vetting ; External collaboration (Corporates digital transformation features)

ICMD® Workspace / Implementation Example

(In support of Corporates Digital Transformation)



IDE can also be deployed within Corporate own private Clouds

Markets / Industrial Innovation Partnerships








QuesTek is presently interacting with Industrial Sectors (Producers, OEM's, End-users) and establishing "Strategic Innovation Partnerships", through collaborations focused on ICME / AIM & ICMD platform to

"…change the way industries do things…"

The QuesTek Difference: in-house Expertise, vetted Experience and proven Track-record

QuesTek's **ICME/AIM** "knowledge, expertise, and experience" are valued globally

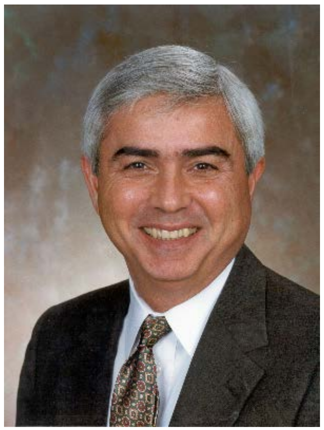
QuesTek Europe AB (Stockholm)

QuesTek is working with entities in Japan

- Optimization of processing to maximize the performance of currently used materials
- Design and development of novel materials at lower cost (reduce risk and accelerate deployment)

QuesTek Japan KK (Tokyo)

THANK You for your attention



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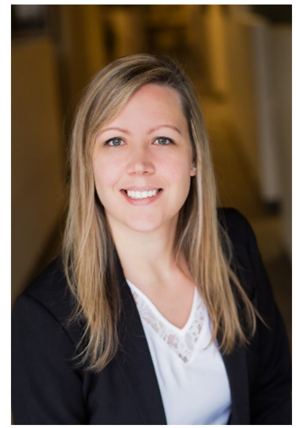

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Appendix

Abstract: Accelerated Development of Advanced Alloys Via Integrated Computational Materials Engineering

Advanced materials are recognized as critical building blocks that drive significant innovations in key sectors (e.g., Automotive, Aerospace, Defense, Energy, Medical).

The advent of Integrated Computational Materials Engineering (ICME) technologies (built on CALPHAD thermodynamics and kinetic databases, along with physics-based models and advanced computational tools) have led to the design and deployment of best-in-class alloys.

Succinct illustration of ICME design steps will be explained, and examples of ICME-designed copper alloys will be provided. Also, projects related to applications of ICME technologies in Additive manufacturing (AM) will be presented.

While Machine Learning and Artificial Intelligence play important role in accelerating the discovery of new materials, the ICME technologies are recognized as essential to the design and deployment of advanced materials. The impact of *Materials Concurrency™* in support of engineering concurrency (combining innovative design and upgraded manufacturing processes with ICME-designed advanced materials) will be highlighted.

The need for integrated materials platforms involving materials informatics (e.g., Data, Models, Tools) to breakdown barriers between materials discovery and their deployment will be addressed, with examples of an Integrated Design Engine platform and its associated software usefulness in predicting the physical properties of AM built parts.

Dr. Aziz Asphahani (QuesTek Innovations-USA)   Dr. Ida Berglund (QuesTek Europe)

2019: 50 Year Anniversary of “foot print” on the moon

Trainer Jet
Ferrium M54 steel
hookshank

Venus Lander
Ferrium C61 steel
gearbox (operate at 900°F)

Mars Space Capsule
Ferrium S53 alloy
components

QuesTek making “ICME/AIM” foot prints on three planets !..

QuesTek Additive Manufacturing Activities (67 AM-related projects)

- **DARPA Open Manufacturing: DMLS of Ni superalloy 718+**
  - Alloy 718+ **Accelerated Process Optimization/AIM-based Component Qualification**
  - Honeywell Aerospace (OEM); ESI Group (AM process modeling); Stratonics and B6 Sigma (AM process monitoring); Southwest Research Institute (UQ)
- **ONR Phase II SBIR "Computational Design of Al-alloy for AM of Gearbox"**
  - Bell Helicopter, Stratasys DM (DMLS), LPW Technology (Powder)
- **Ti alloy development for additive manufacturing**
  - Development of QuesTek's castable titanium alloys (Army SBIR) for AM
  - Lockheed Martin (OEM); Sciaky (EBAM process)
- **Air Force MAI "ICME Development for Additive Manufactured/Aerospace"**
  - High-temperature Ti and Ni alloys
  - Honeywell, Lockheed Martin, Rolls-Royce, Aerojet Rocketdyne (OEMs); Carpenter Technology and ATI Powder Metals; Applied Optimization
- **Navy Phase I SBIR "Development of 7050 Al Alternative for AM"**
  - Boeing Vertical Lift and Northrop Grumman (OEMs), Stratasys DM (DMLS)

ICME-Designed Materials for Additive Manufacturing

Ferrium C64® powder

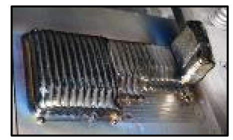
EBAM

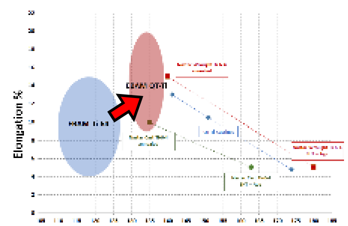
DMLS

Additive C64 meets static mechanical property minima, exceeding that of incumbent wrought alloys (e.g., Alloy X53)

Mod Ti-6-4 alloy

- ***Enhanced properties***
- ***Improved reproducibility***
- ***Adaptable to recycling***





ICME-designed Hi-temp Al-alloy