

ASETSDefense 2011: Sustainable Surface Engineering for Aerospace and Defense Workshop

February 8-10, 2011

New Orleans, LA



Materials by Design - Computational Alloy Design for Corrosion



Charlie Kuehmann

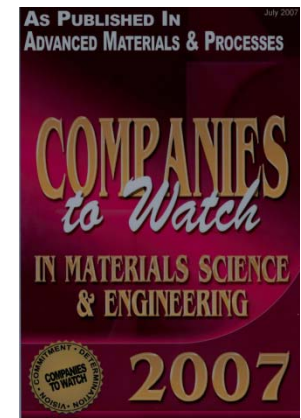
QUESTEK[®]
INNOVATIONS LLC
Materials By Design[®]

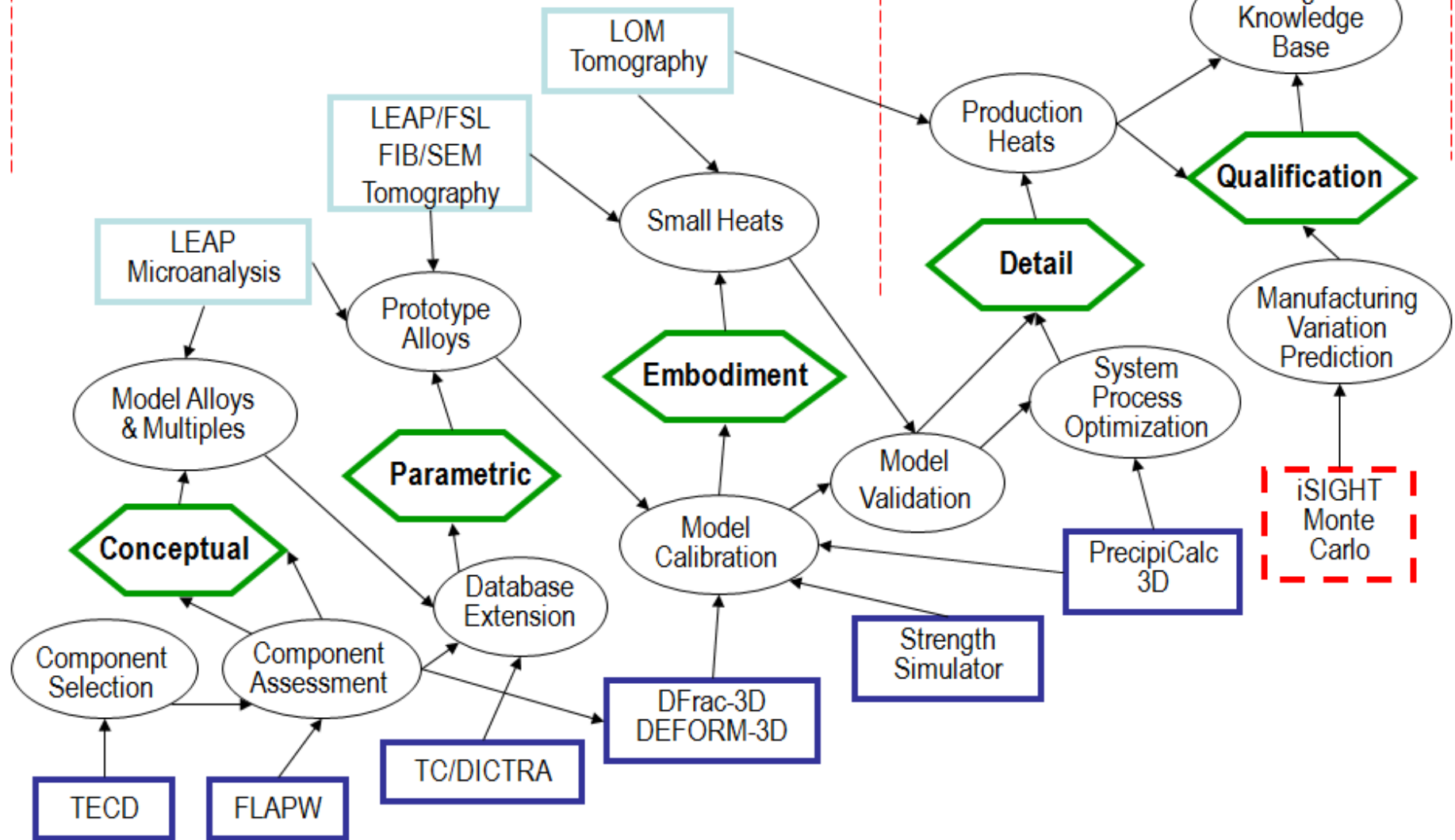
www.questek.com

Report Documentation Page				Form Approved OMB No. 0704-0188	
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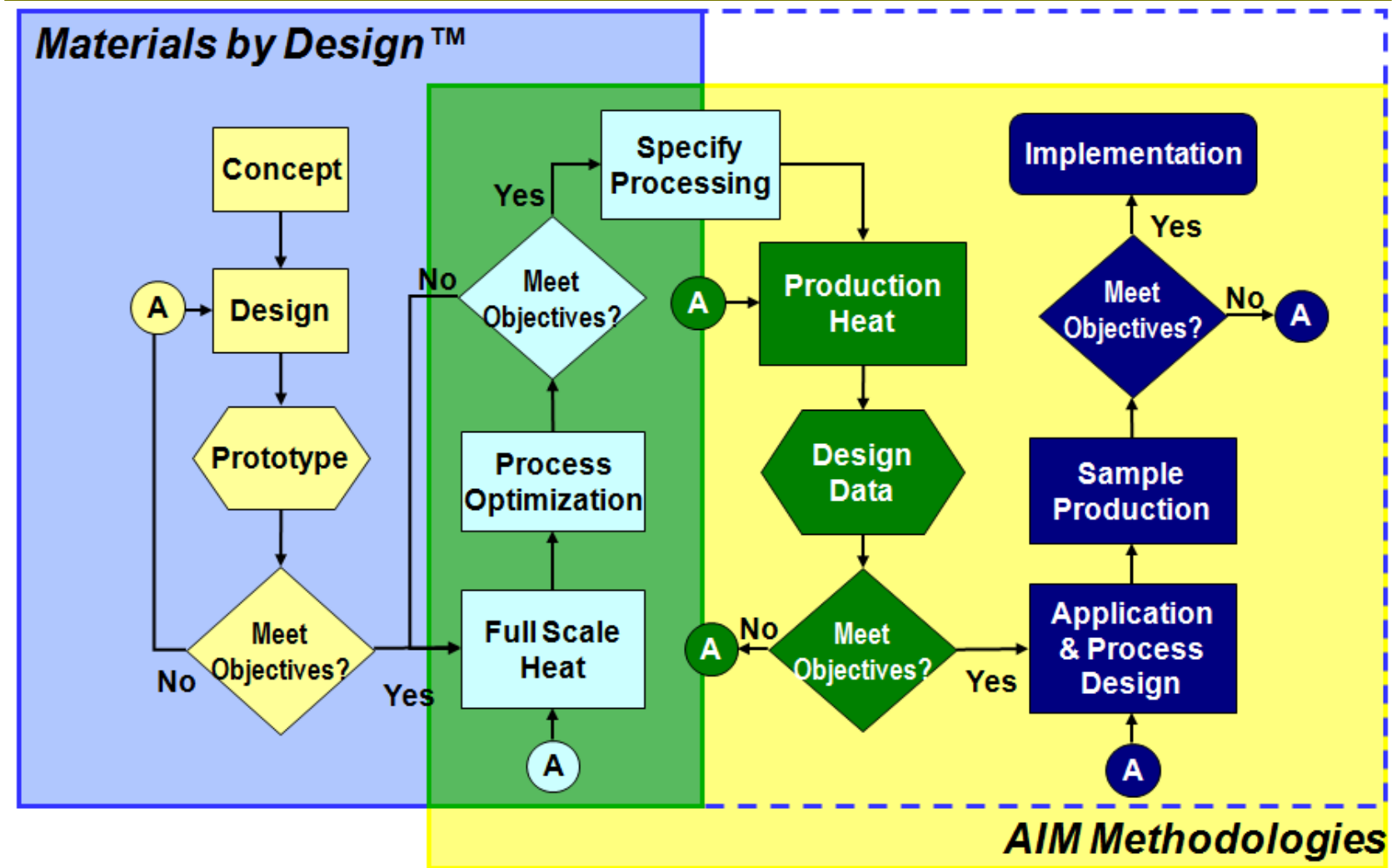
Background - QuesTek Innovations LLC

- 16 engineers, 9 with PhDs; founded 1997
- Rapidly designing, developing, qualifying and inserting new materials using computational methods on integrated basis
- Creates IP; licenses to OEMs or alloy producers/processors
- 4 alloys licensed: *Ferrium*® M54™, C61™, C64™ and S53®
- Working with many colleagues in industry and academia
- ~10 major new alloys in development
- 30+ patents awarded or pending worldwide
- Serving industry and government
- Recipient of many business and technology awards
- Expanding our staff

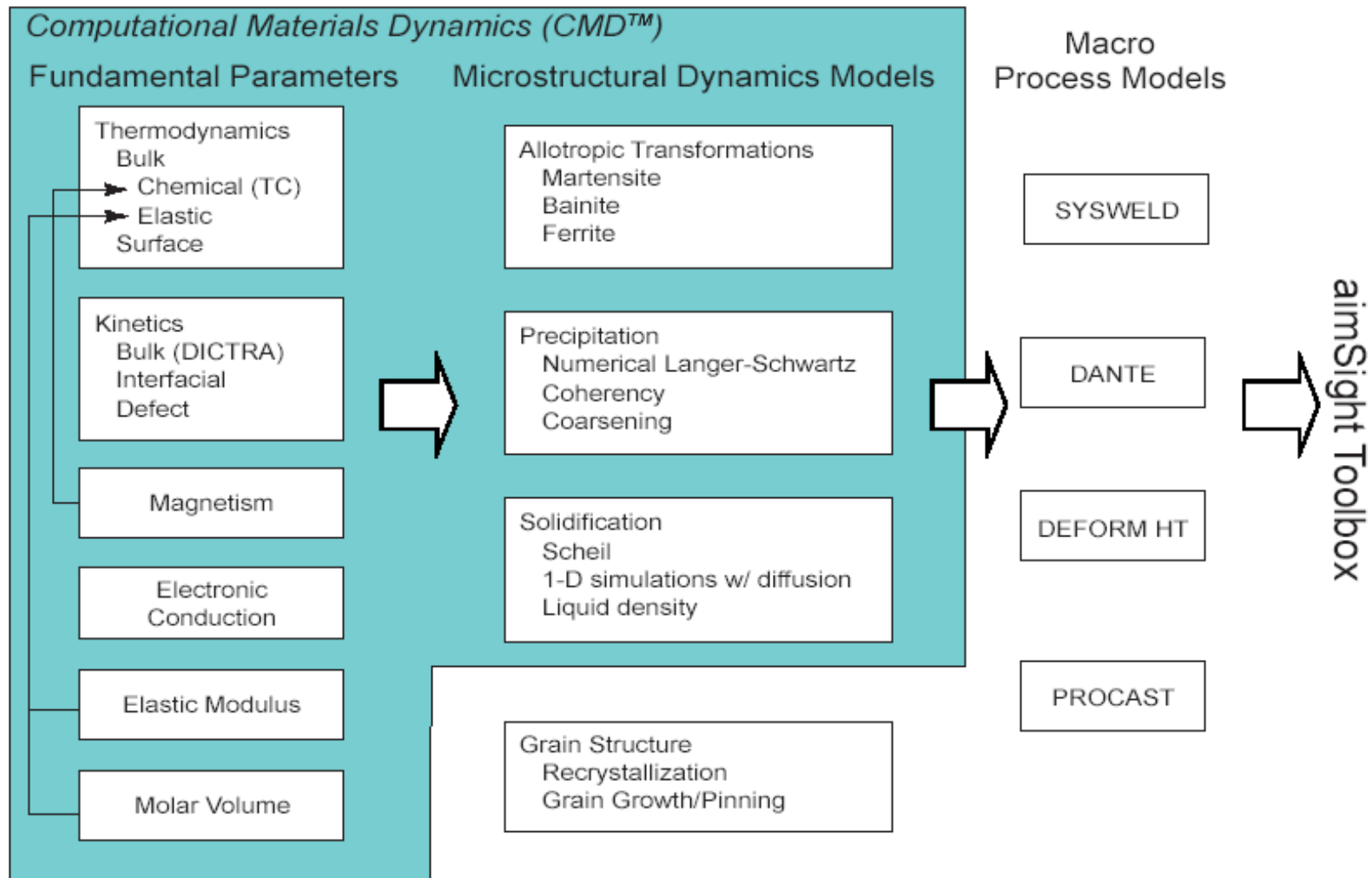




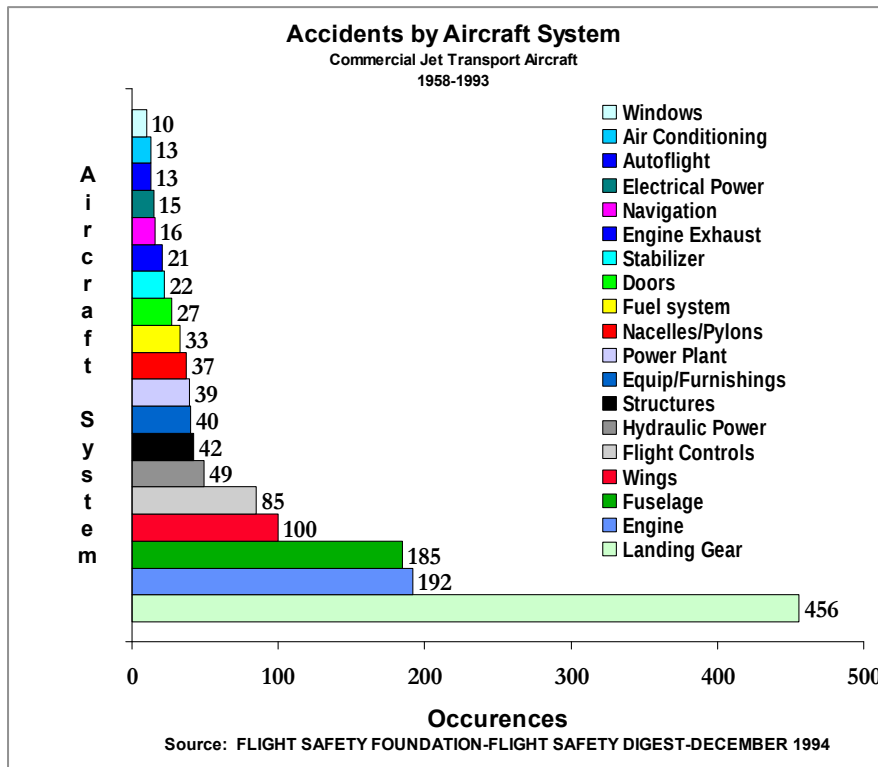
Accelerating the Materials Development Cycle



Process-Structure Modeling



A First Example of Materials Design for Corrosion



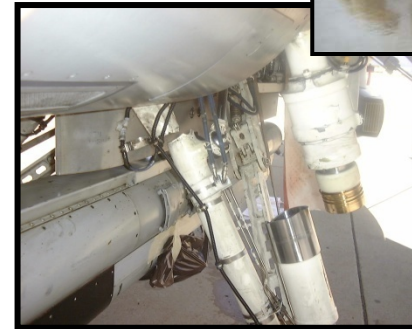
Issues:

Over \$200 million spent in LG per year
80% corrosion related

SCC failures

Cad plating used to protect current steel
known carcinogen (Hill AFB ~ 2000 lbs/yr)

SCC failures



HE failures

Benefits:

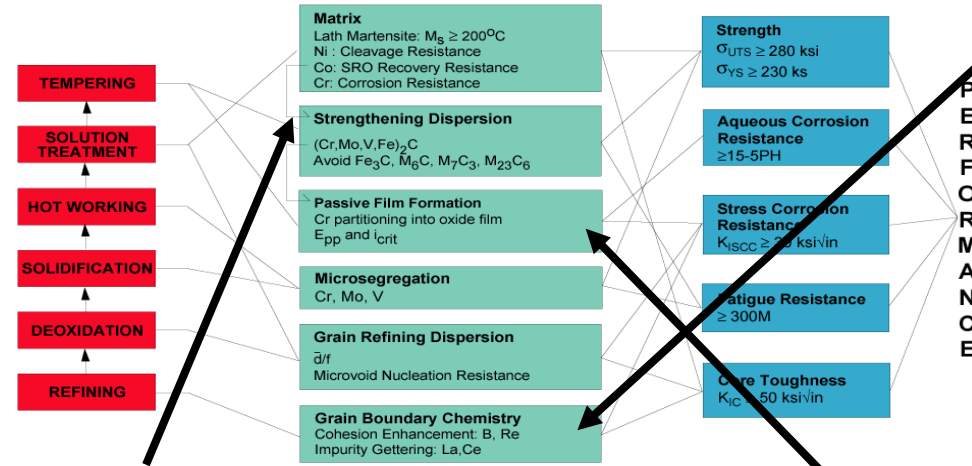
Dramatic reduction in LG cost (60%)
savings of \$120 million per year
Significant reduction in SCC failures
Cadmium plating not required
General corrosion mitigated
80% of Steel Condemns Avoided

Design Models Founded on Scientific Understanding but Implemented for Optimization

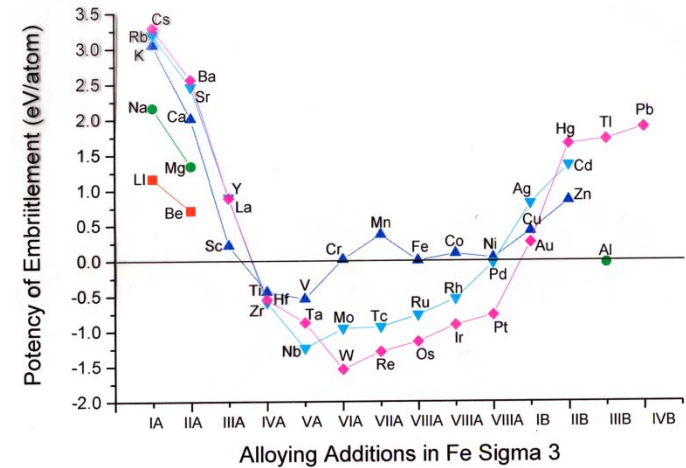
PROCESSING

STRUCTURE

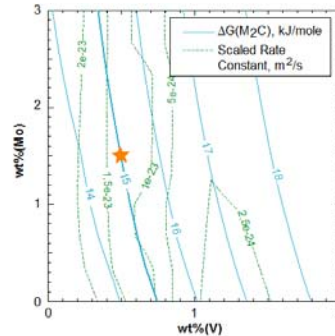
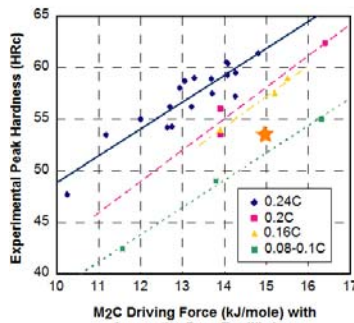
PROPERTIES



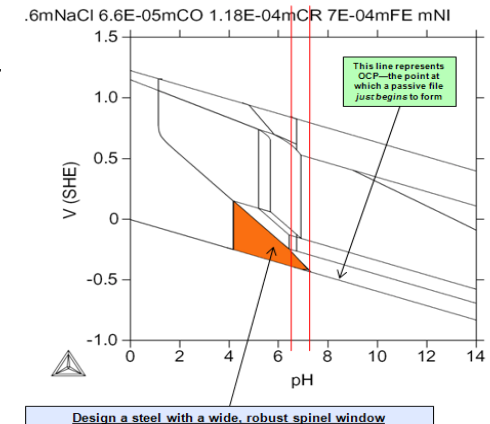
Chris Kantner - "Quantum Steel"
PhD thesis Northwestern, 2001



Charlie Kuehmann - "Thermal Processing Optimization of Nickel-Cobalt Ultra High-Strength Steels"
PhD thesis Northwestern, 1994



Carelyn Campbell - "Systems Design of Stainless Bearing Steel"
PhD thesis Northwestern, 1996



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Corrosion modeling

Pourbaix diagrams

Design a steel with a wide, robust spinel window

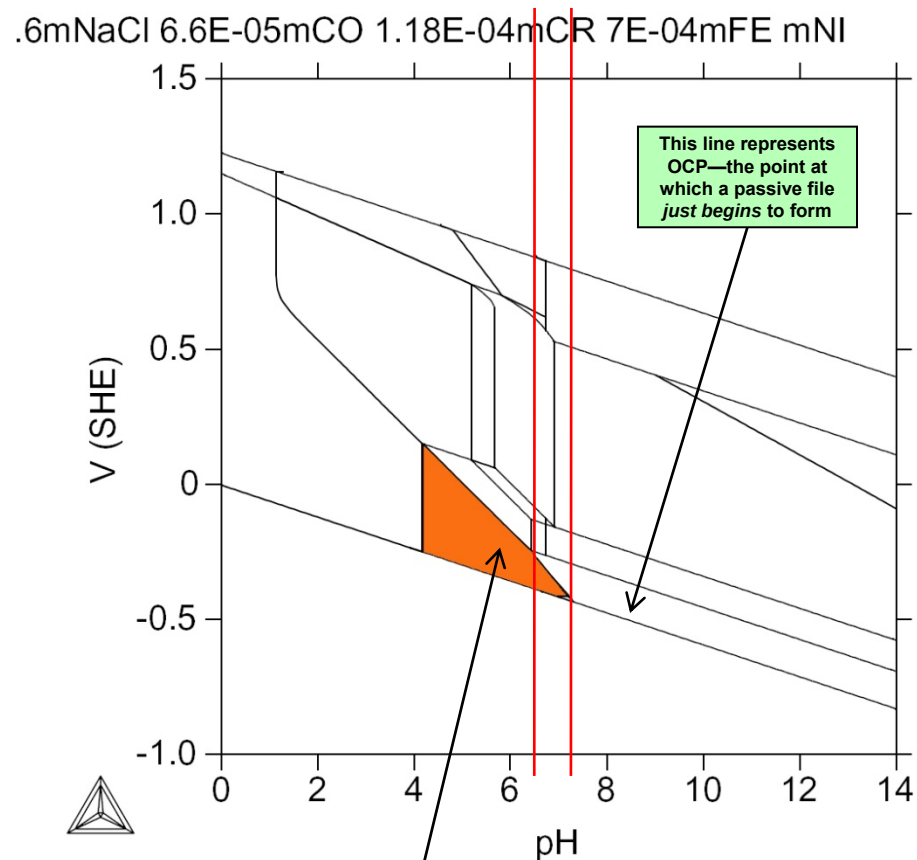
ASTM B117 pH $\approx$ 6.5-7.2

Diagrams not very sensitive to composition

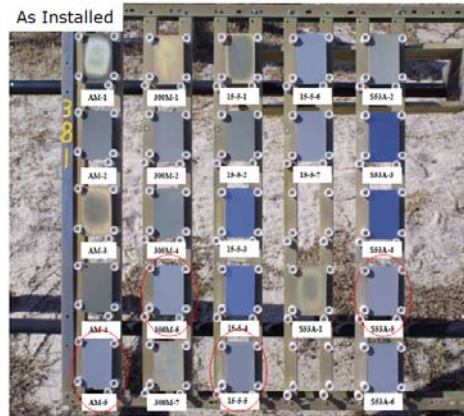
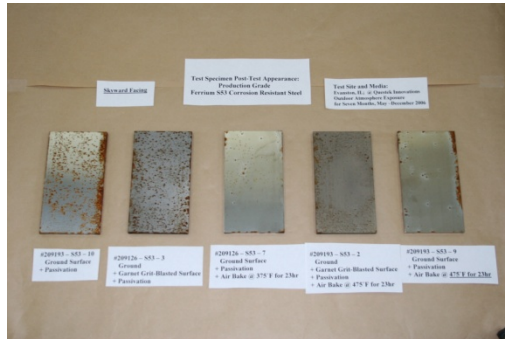
Revised oxide TDB

On the “oxide formation” side of things

Equilibrium

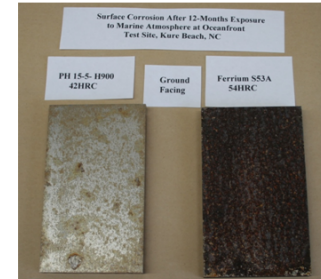


S53 Corrosion Behavior

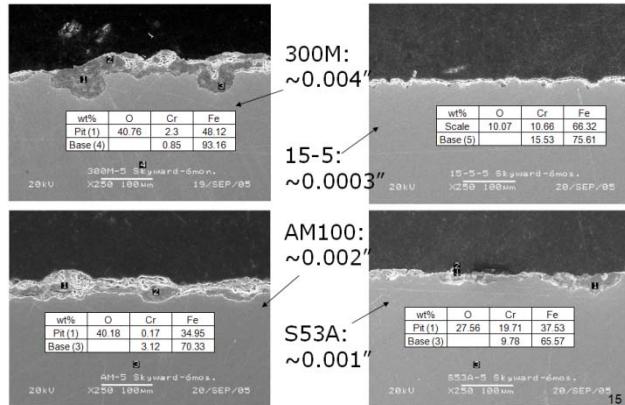


Initial Studies: 12 months
 PH 15-5 (195 ksi) S53A (285 ksi)
 ~0.0005" 0.001" ~0.002"
 pit depth pit depth

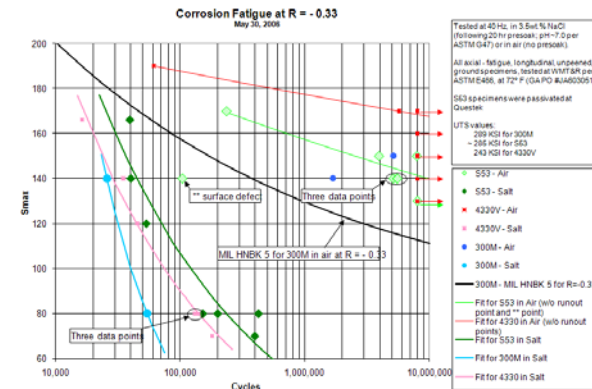
Follow-up Studies: 3 months
 S53 (AMS 5922) (288 ksi)
 0.001" ~0.002"
 pit depth



Exposure tests at QuesTek (left) and Kure beach (center, right)

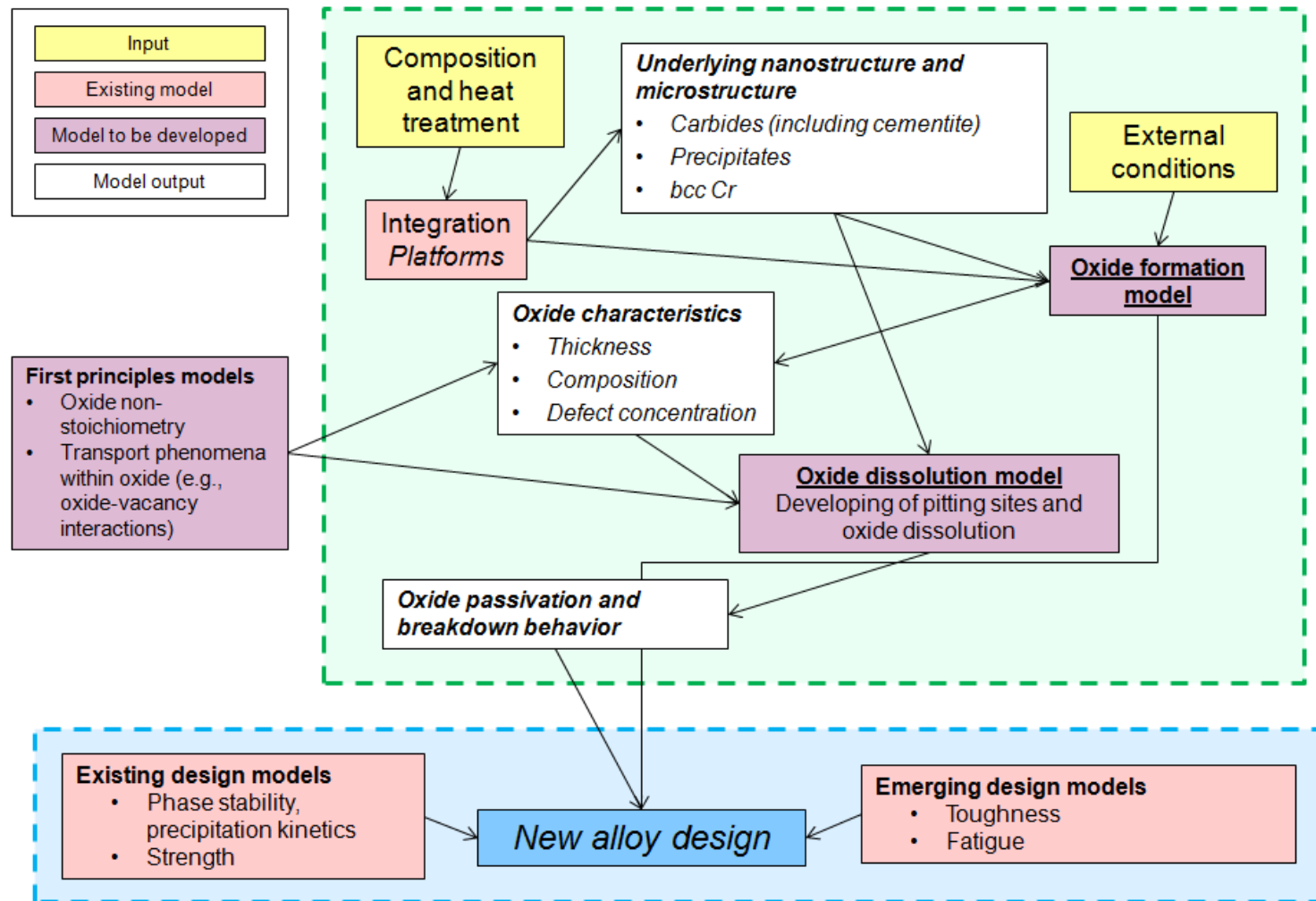


Characterization of corrosion pits

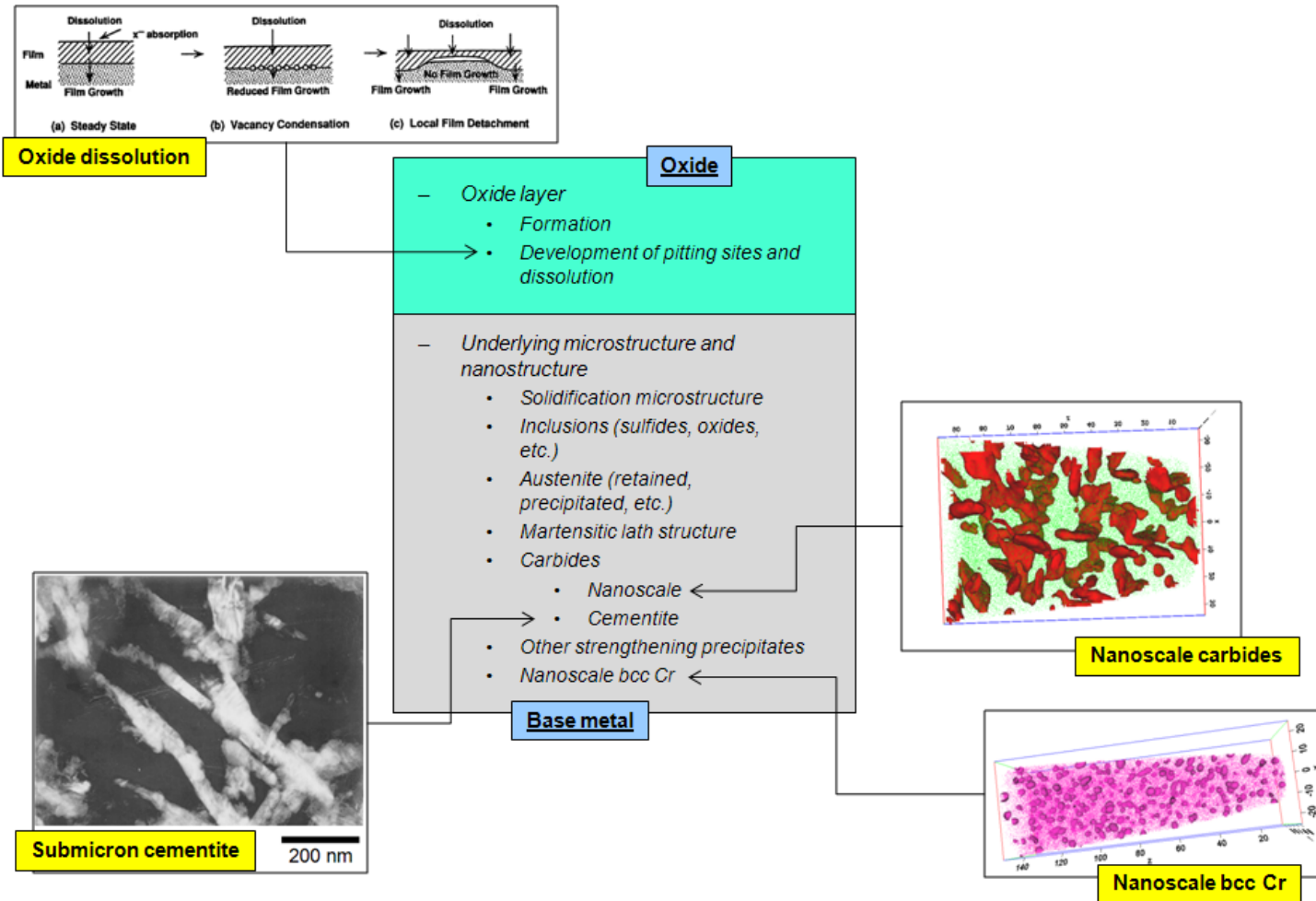


Corrosion fatigue testing

A Corrosion Modeling Architecture

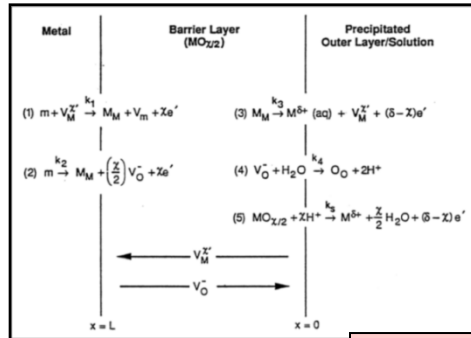


Multiscale representation of the metal/oxide system

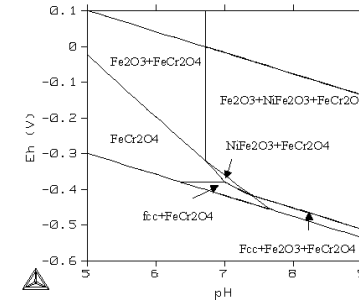
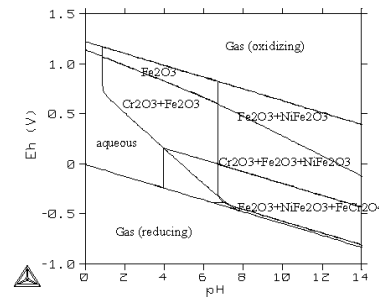


Oxide formation and dissolution

Oxide formation (PDM framework, left;)

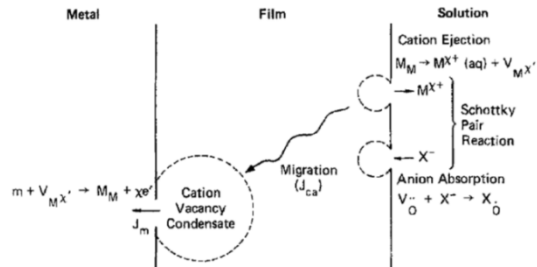


Oxide formation

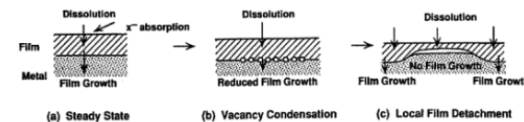


Calculated Pourbaix diagrams

Oxide dissolution (PDM framework)



Cation condensation



Repassivation

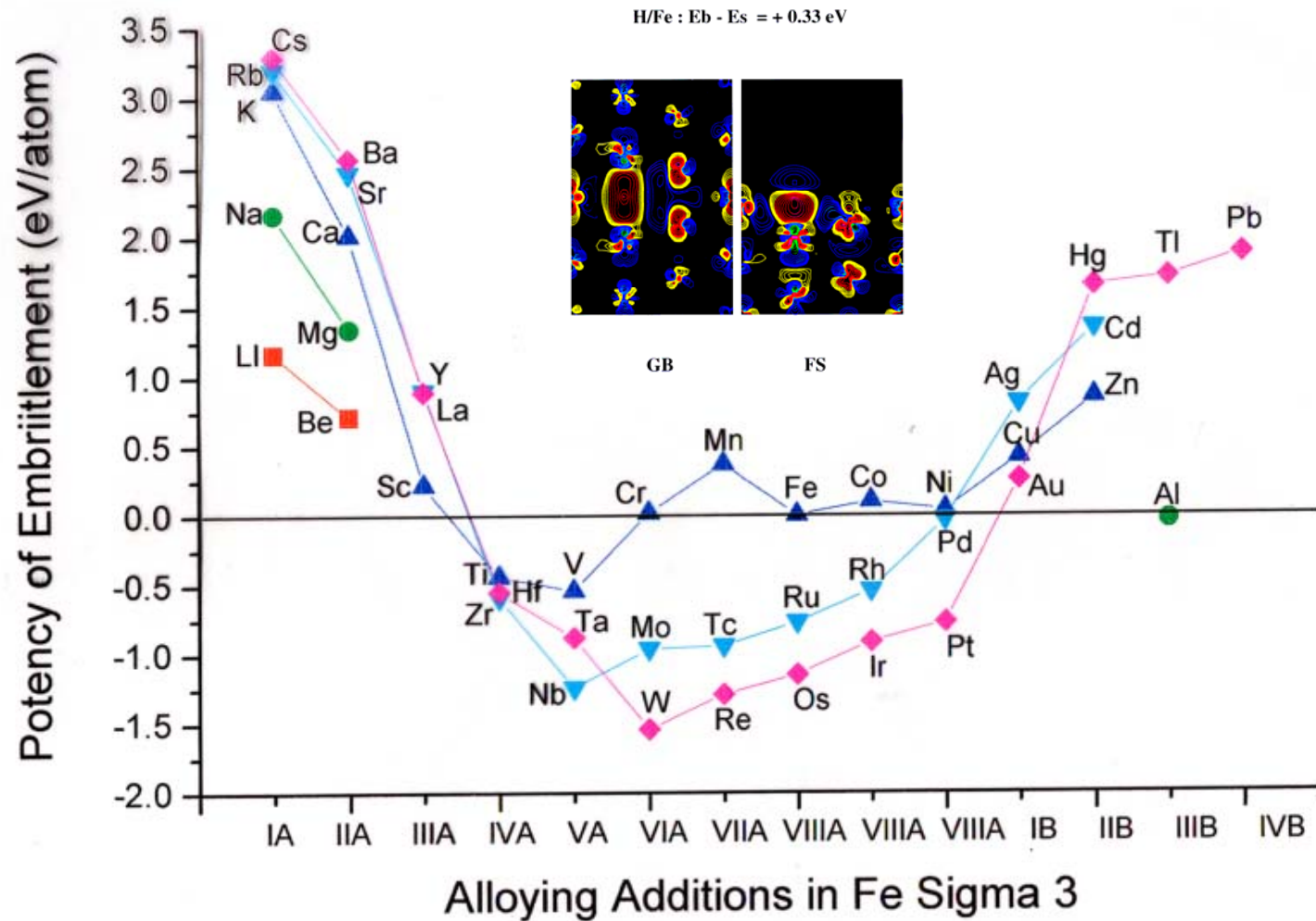
Stable Pit Growth

Oxide dissolution and rupture

Figures from D.D. Macdonald, *Pure and Applied Chemistry*, 71(6),

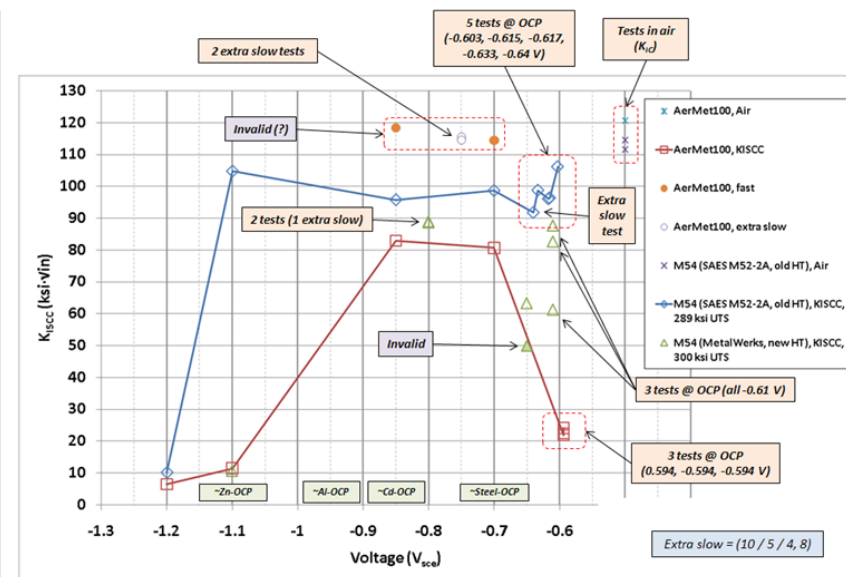
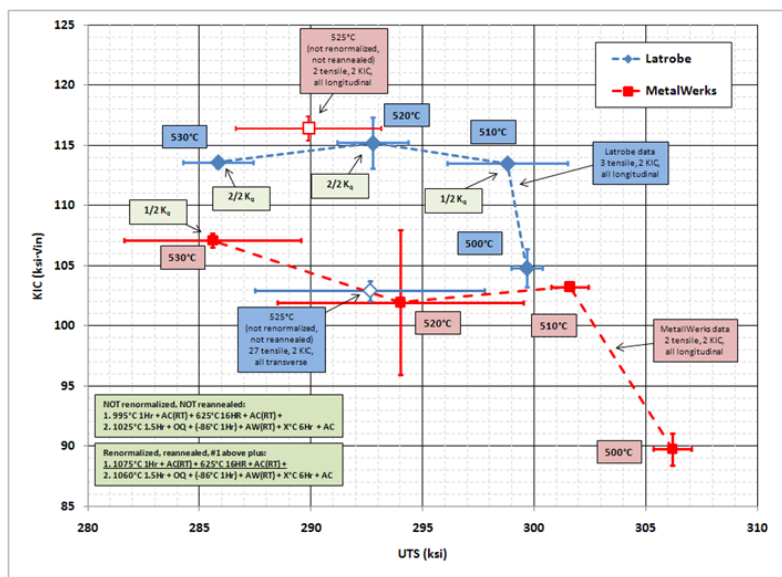
1993

Quantum Mechanics Insights into SCC resistance

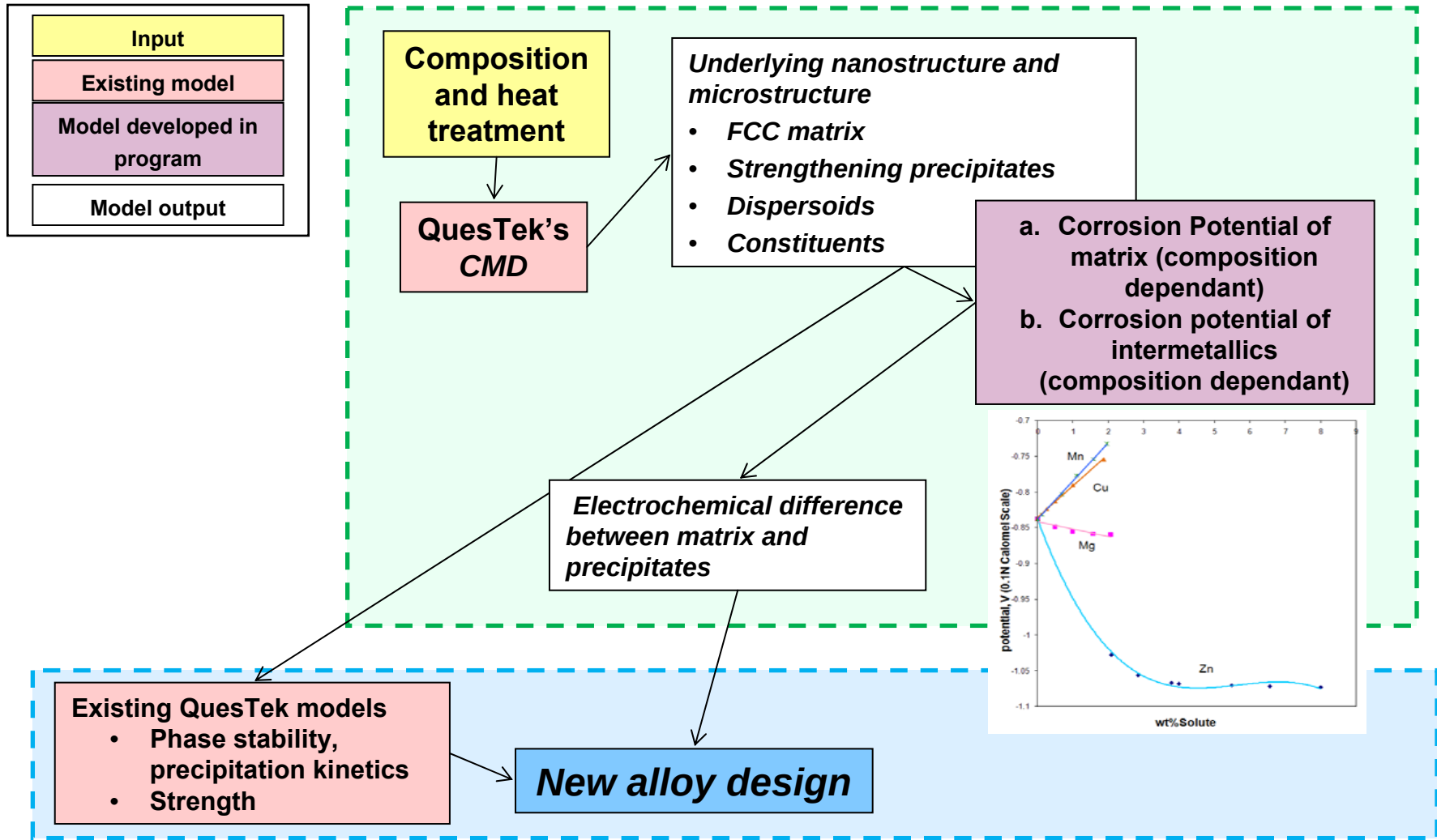


Example: Lower Cost Designs for Optimal SCC Resistance

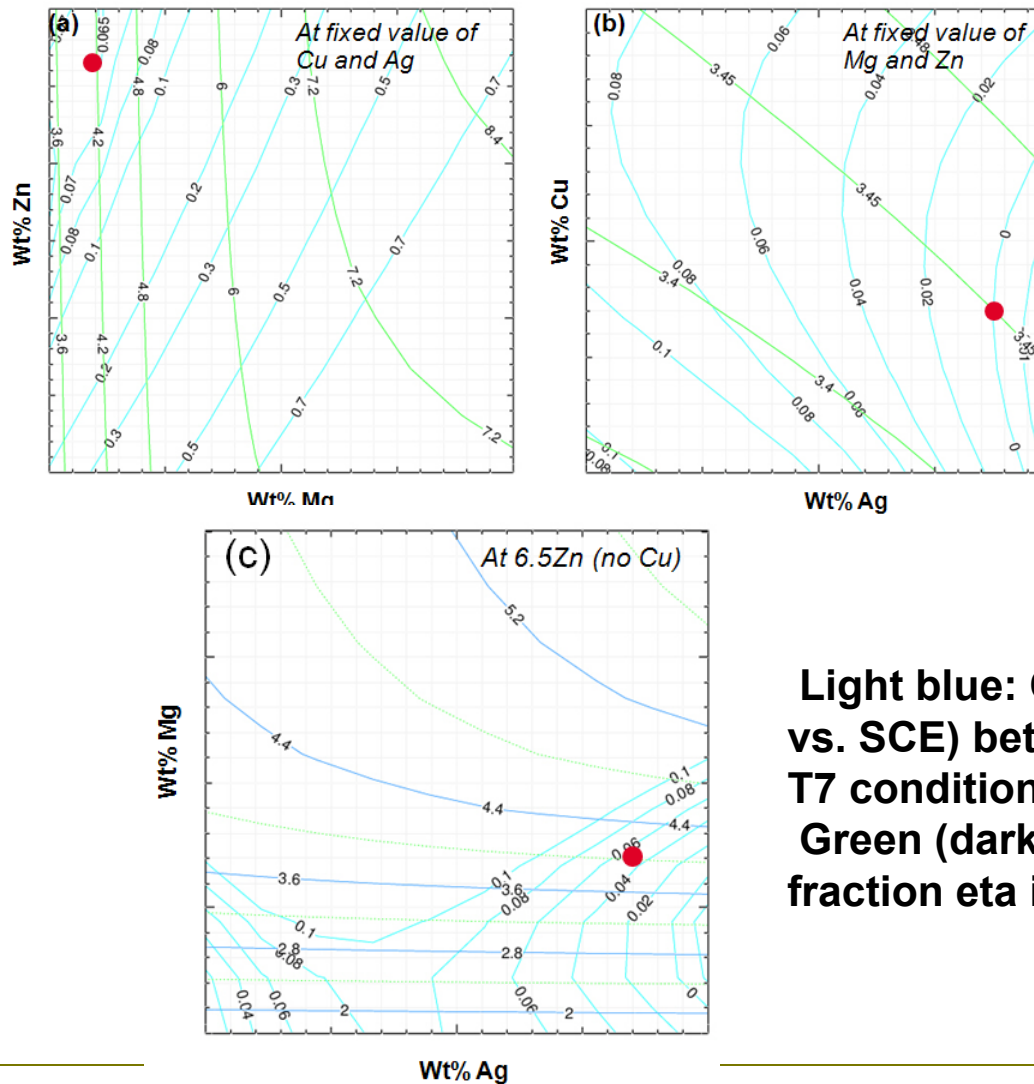
- *Ferrium M54*
 - Navy SBIR program
 - Navy SBIR topic N07-032, “Computational Design of Advanced Alloys for USN Landing Gear.” Currently in Phase II (contract N68335-08-C-0288). TPOCs Amy Little and Michael Leap.
 - Phase I: 2007-2008
 - Phase II Base: 2008-2010
 - Full-scale production, demonstration of 1% minimum properties, patented composition with commercial licensee



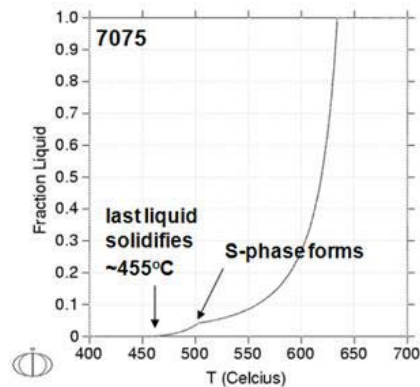
Schematic of an electrochemical framework



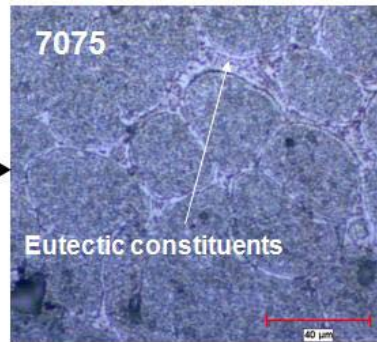
QuesTek “OCP” designs utilizing implemented models



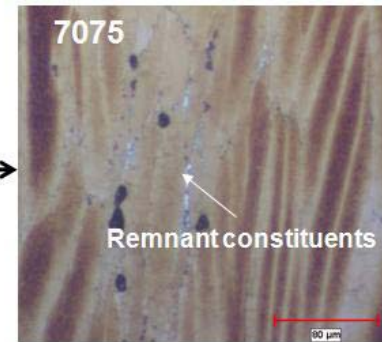
Simulated solidification curves and experimental micrographs for alloy 7075 and QuesTek alloy Al-1B



Solidification simulations for 7075 and QuesTek Al-1B alloy

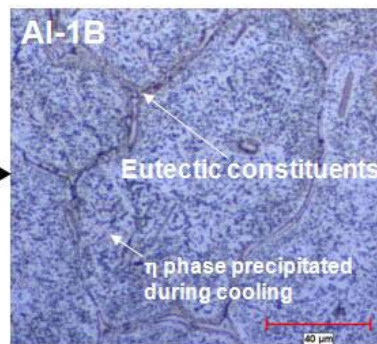
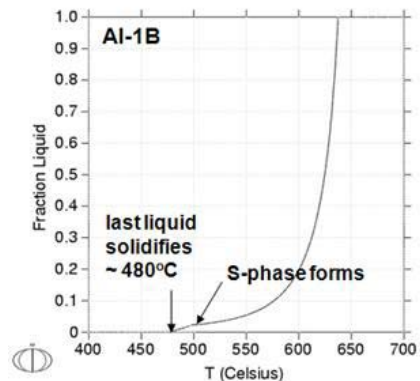


As-cast + stress-relieved microstructure



Homogenized + T73 heat-treated microstructure

White:
Undissolved S-phase/eta
Black: $\text{Al}_7\text{Cu}_2\text{Fe}$



Fully dissolve soluble solidification constituents by selecting optimal solidification behavior and optimal homogenization treatment

D 3-D digital structure

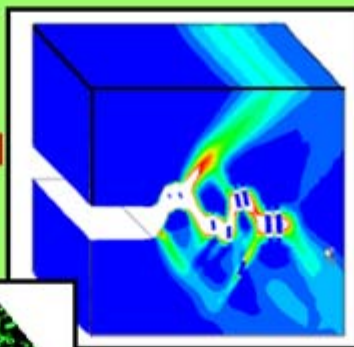


Design Research Tools



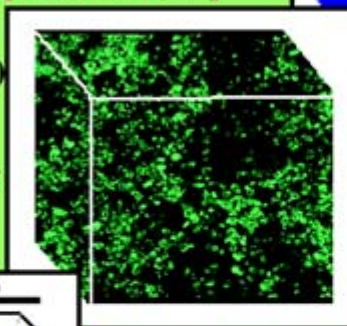
matCAT Characterization & Visualization Toolset

LOM
Tomography
[Olson, Voorhees]
Toughness,
Fatigue Strength
[Olson, Kern]



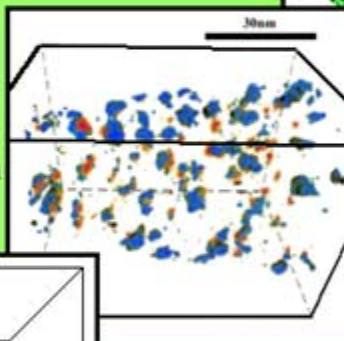
Ductile
Fracture
[Moran,
Liu, Parks]
Fatigue
Nucleation
[McDowell,
Olson]

FSL(SEM/TEM)
Tomography
[Pollock]
Shear Instability
[Olson, Kern]

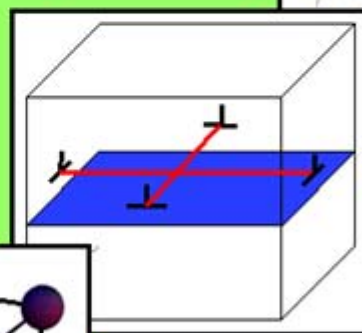


Microvoid Shear
[Moran, Liu, Parks]
Fatigue Propagation
[McDowell]

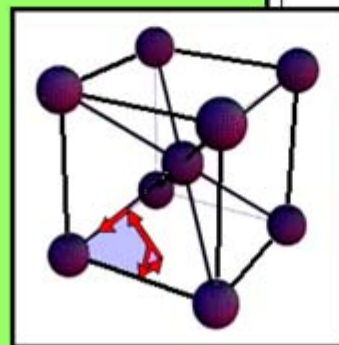
LEAP
Tomography
[Seidman]
Yield Strength
[Olson, Kern]



Transformation
Toughening
[Parks, Olson]
Precipitation
Strengthening
[Voorhees,
Wang, Jou]



Semicoherent IPB
Adhesion
[Freeman,
Jerome, Wang]



Bond Topological
S/P Relations
[Eberhart]

TECD

FLAPW

PrecipiCalc-3D

DFrac-3D

iSIGHT/CMD Integration

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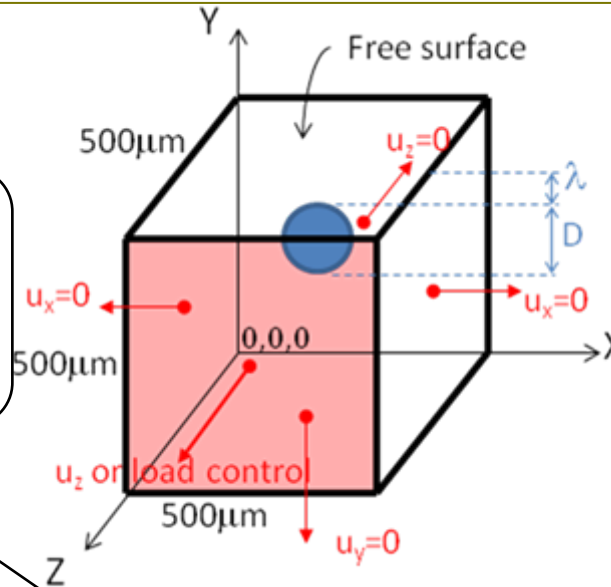
Input to Microstructure-Sensitive Fatigue Life Prediction

Microstructure:

- partially debonded NMP (Al_2O_3), intact NMP (Al_2O_3), or pore; distances to free surface, size extremes (from *)
- mesh — grain size, orientation

FEM Model:

- $(500\mu\text{m})^3$ box
- one embedded anomaly
- one free surface
- loading or displacement control along z-axis

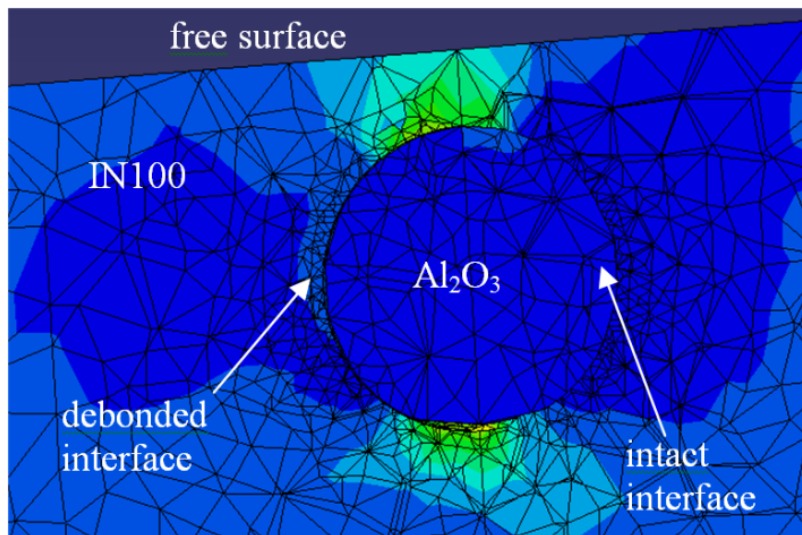


Test Conditions (from *):

- $\sigma=1100$ or 1200MPa
- $T=650^\circ\text{C}$
- $R=0.05$

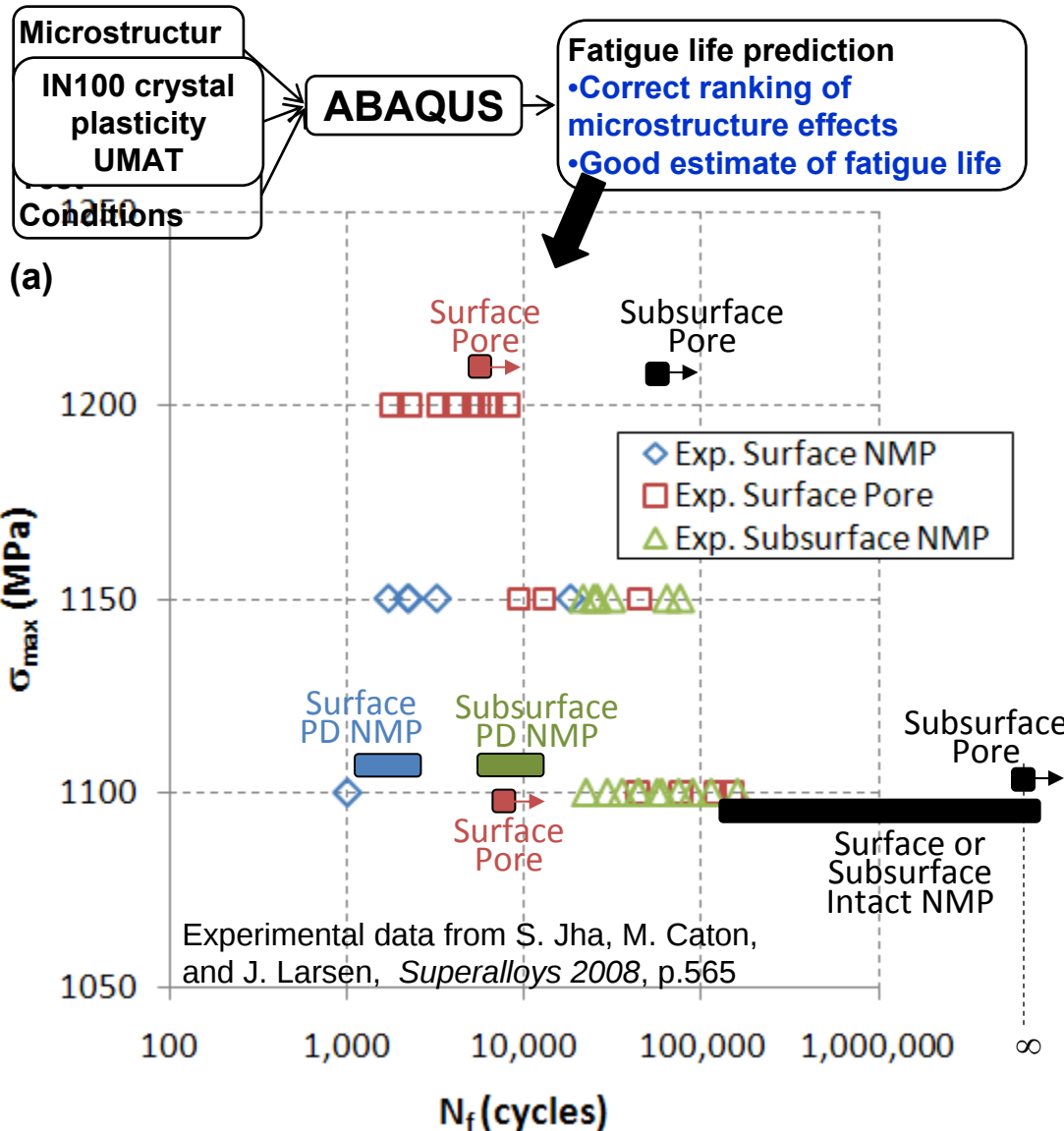
IN100 crystal plasticity UMAT developed by GIT under DARPA AIM

ABAQUS cyclic loading simulations

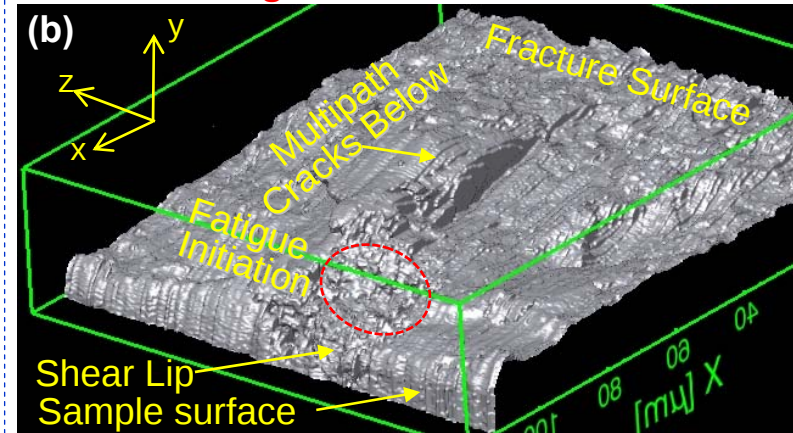


* S. Jha, M. Caton, and J. Larsen, *Superalloys 2008*, p.565

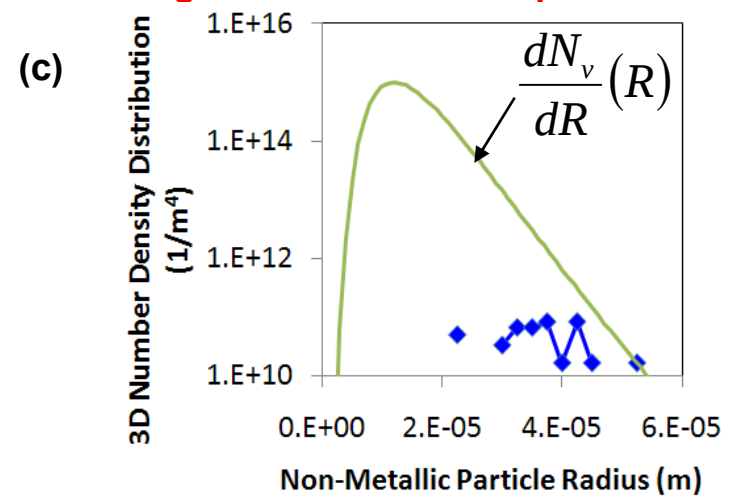
- Demonstrated feasibility of microstructure-sensitive fatigue simulation and fatigue life prediction**



- 3D Tomographic Reconstruction Illustrated Microstructure Features Around Fatigue Initiation Site**



- Synthesized fractographic and metallographic data for NMP/pores**



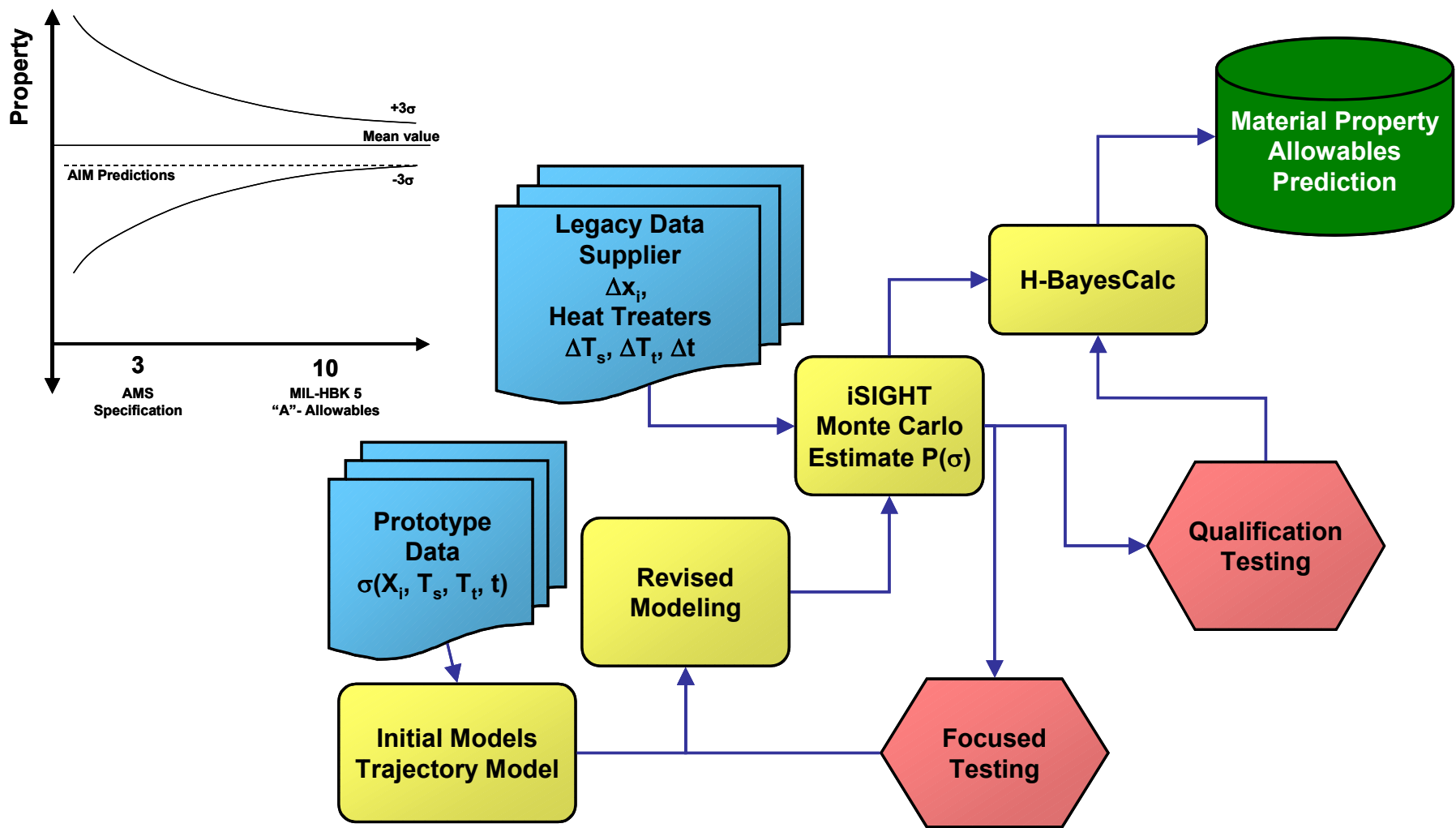
- Developed approaches to incorporate dwell effects in transition zone**

Material Qualification

- SAE – Aerospace Materials Specification (AMS)
 - This is the material procurement document
 - Data: 3 heats, 30 tensile, 30 fracture toughness
 - Analysis/approval by Battelle Memorial
 - Document: draft an AMS document
 - Approval by AMS subcommittee
 - Approval by AMS – Aerospace Council
- Metallic Material Properties Development and Standardization (MMPDS)
 - This is the design allowables document
 - Data: 10 heats, 100 tensile, 30 fracture toughness, 20 compression, 20 shear, 20 pin bearing ($e/D = 1.5, 2.0$), physical properties, etc..
 - Analysis by Battelle Memorial
 - Approval by MMPDS committee and FAA



Accelerating the Qualification Cycle

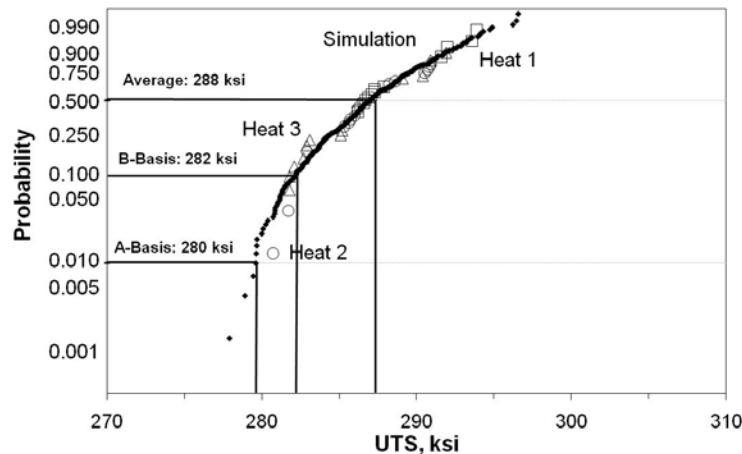




AIM Application Example: Ferrium S53®

Data generated for 3 melts/Simulations for 10

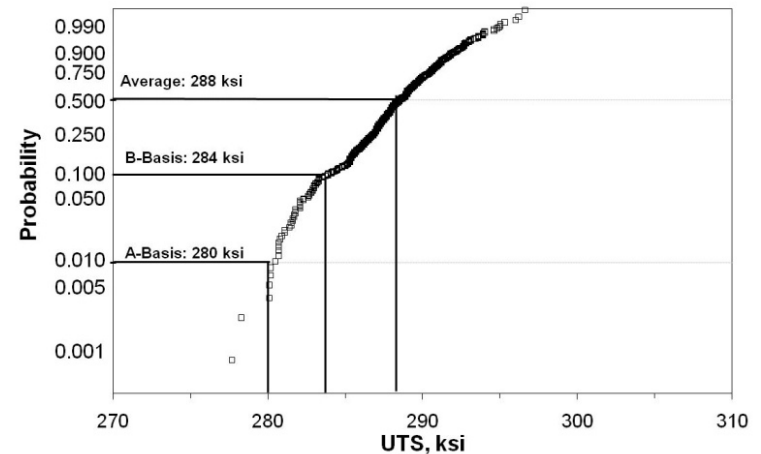
- Predicted A-basis minimum = 280 ksi UTS



Full Data
Development

Data generation for 10 melts

- A-basis minimum: 280 ksi UTS



- AIM has demonstrated reliable predictions for design minimums
- Allows designers to consider alloys prior to full design allowable development
- Reduce costs and risks for material design and development

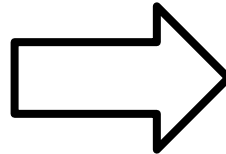
Flying Cybersteels

- S53 Field service evaluation (approved August, 2010)
 - 6 to 24 months in test to determine preventative maintenance cycles



Experience lets us expand to new platforms ...

Original Demonstrations

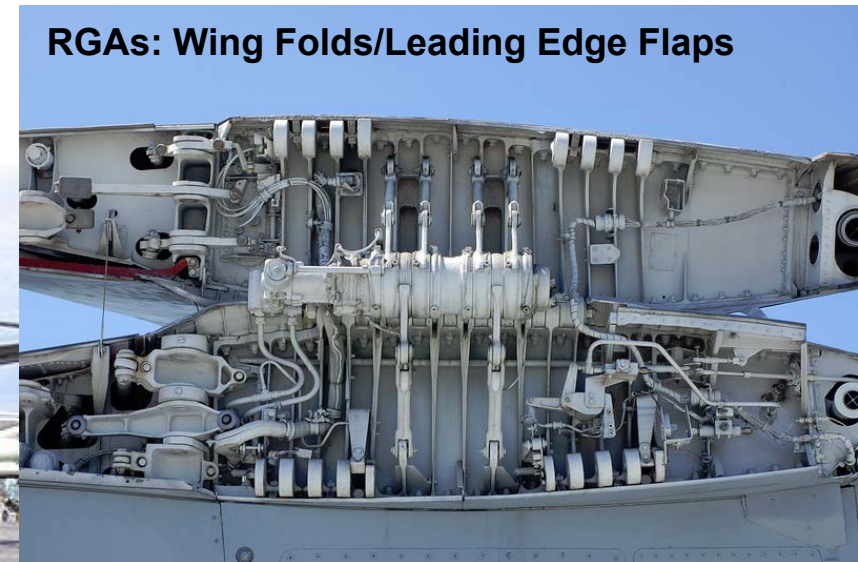


New Platforms



... and to new applications

Capability extensions such as new surface hardening processes allow us to explore applications where life is limited by wear...



The next frontier...

hydrogen 1 H 1.0079																		helium 2 He 4.0026																			
lithium 3 Li 6.941		beryllium 4 Be 9.0122																		boron 5 B 10.811		carbon 6 C 12.011		nitrogen 7 N 14.007		oxygen 8 O 15.999		fluorine 9 F 18.998		neon 10 Ne 20.180							
sodium 11 Na 22.990		magnesium 12 Mg 24.305																		aluminum 13 Al 26.982		silicon 14 Si 28.086		phosphorus 15 P 30.974		sulfur 16 S 32.065		chlorine 17 Cl 35.453		argon 18 Ar 39.948							
potassium 19 K 39.098		calcium 20 Ca 40.078		scandium 21 Sc 44.956		titanium 22 Ti 47.867		vanadium 23 V 50.942		chromium 24 Cr 51.996		manganese 25 Mn 54.938		iron 26 Fe 55.845		cobalt 27 Co 58.933		nickel 28 Ni 58.693		copper 29 Cu 63.546		zinc 30 Zn 65.39		gallium 31 Ga 69.723		germanium 32 Ge 72.61		arsenic 33 As 74.922		selenium 34 Se 78.96		bromine 35 Br 79.904		krypton 36 Kr 83.80			
rubidium 37 Rb 85.468		strontium 38 Sr 87.62		yttrium 39 Y 88.906		zirconium 40 Zr 91.224		niobium 41 Nb 92.906		molybdenum 42 Mo 95.94		technetium 43 Tc [98]		ruthenium 44 Ru 101.07		rhodium 45 Rh 102.91		palladium 46 Pd 106.42		silver 47 Ag 107.87		cadmium 48 Cd 112.41		indium 49 In 114.82		tin 50 Sn 118.71		antimony 51 Sb 121.76		tellurium 52 Te 127.60		iodine 53 I 126.90		xenon 54 Xe 131.29			
caesium 55 Cs 132.91		barium 56 Ba 137.33		57-70 ✱		lutetium 71 Lu 174.97		hafnium 72 Hf 178.49		tantalum 73 Ta 180.95		tungsten 74 W 183.84		rhenium 75 Re 186.21		osmium 76 Os 190.23		iridium 77 Ir 192.22		platinum 78 Pt 195.08		gold 79 Au 196.97		mercury 80 Hg 200.59		thallium 81 Tl 204.38		lead 82 Pb 207.2		bismuth 83 Bi 208.98		polonium 84 Po [209]		astatine 85 At [210]		radon 86 Rn [222]	
francium 87 Fr [223]		radium 88 Ra [226]		89-102 ✱ ✱		lawrencium 103 Lr [262]		rutherfordium 104 Rf [261]		dubnium 105 Db [262]		seaborgium 106 Sg [266]		bohrium 107 Bh [264]		hassium 108 Hs [269]		meitnerium 109 Mt [268]		ununilium 110 Uun [271]		unununium 111 Uuu [272]		ununbium 112 Uub [277]		ununquadium 114 Uuq [289]											

* Lanthanide series

** Actinide series

lanthanum 57 La 138.91	cerium 58 Ce 140.12	praseodymium 59 Pr 140.91	neodymium 60 Nd 144.24	promethium 61 Pm [145]	samarium 62 Sm 150.36	europium 63 Eu 151.96	gadolinium 64 Gd 157.25	terbium 65 Tb 158.93	dysprosium 66 Dy 162.50	holmium 67 Ho 164.93	erbium 68 Er 167.26	thulium 69 Tm 168.93	ytterbium 70 Yb 173.04
actinium 89 Ac [227]	thorium 90 Th 232.04	protactinium 91 Pa 231.04	uranium 92 U 238.03	neptunium 93 Np [237]	plutonium 94 Pu [244]	americium 95 Am [243]	curium 96 Cm [247]	berkelium 97 Bk [247]	californium 98 Cf [251]	einsteinium 99 Es [252]	fermium 100 Fm [257]	mendelevium 101 Md [258]	nobelium 102 No [259]

Using ICME to Significantly Improve Equipment Performance, Affordability and EHS

Marine Corps: M67854-05-C-0025



Army: W15QKN-09-C-0026



Navy: N65538-09-M-0088



NAVAIR: N68335-07-C-0302 and N68335-08-C-0288



ONR: N00014-05-M-0250
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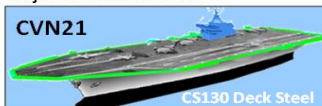
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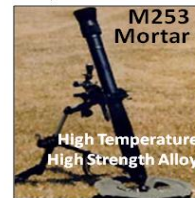
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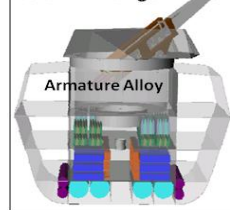
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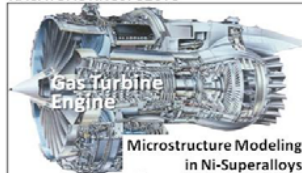
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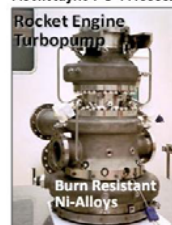
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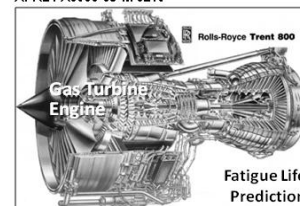
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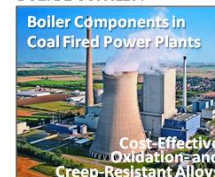
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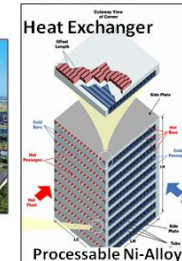
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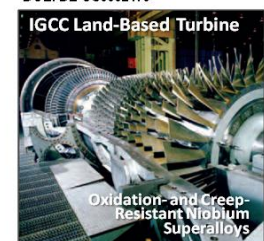
DOE: DE-SC0002234



NSF IIP-0839678



DOE: DE-SC0002475



Thank You

Questions?

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