From Genome to Flying Cyberalloys: The First Half Century

G. B. Olson
Northwestern University

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From Genome to Flying Cyberalloys: The First Half Century

G.B. Olson
Northwestern University & QuesTek Innovations LLC
Evanston, Illinois
Fundamental databases and tools enabling reduction of the 10-20 year materials creation and deployment cycle by 50% or more.
Chapter 3, p. 42:
A productive model may be the health-driven research system operated by the National Institutes of Health, spanning the full range from molecular biology to medicine. While the academic value system of the physical sciences has generally suppressed the creation of engineering databases, the life sciences have forged ahead with the Human Genome project representing the greatest engineering database in history. A parallel fundamental database initiative in support of computational materials engineering could build a physical science/engineering link as effective as the productive life science/medicine model.

Recommendation: The Office of Science and Technology Policy should lead a national, multiagency initiative in computational materials engineering to address three broad areas: methods and tools, databases, and dissemination and infrastructure.
First Flight: QuesTek *Ferrium S53® T-38* main landing gear piston
December 17, 2010

Material approval: November 2009
Component approval: August 2010
Component installation: November 2010
First flight: December 2010
Materials Genome Timeline

Integrated Computational Materials Engineering

Computational Materials Design

Ferrous Alloys
Ni-base Alloys
Refractories
SMAs
Cu-base Alloys
Polymers
Ceramics
Composites

Ferrium C61™
Ferrium S53®
Ferrium C64™
Ferrium M54™

1956 Kaufman & Cohen
1973 CALPHAD
1979-84 Thermo-Calc SGTE
1990s DICTRA Pandat Thermotech
2000s DFT Integration

1985 SRG Systems Approach
1989 NASAlloy
1997 Ferrium C61™
2000 Ferrium S53®
2004 Ferrium C64™
2007 Ferrium M54™

2001 DARPA AIM
2003 Ford VAC
2005 DARPA/ONR D3D
2004 NMAB Accelerating Technology Transition
2008 NMAB ICME
2011 OSTP
2011 Materials Genome Initiative

Gen I
Gen II
Gen III

1950
1970
1980
1990
2000
2010
STRUCTURE - C.S. Smith

INTERACTIVE HIERARCHY
- Space-Filling Aggregates: materials science, biology, geology
- Perfection/Imperfecton
- Entity/Identity
- "Mesoscopic" Regime

REAL COMPLEXITY VS. IDEALIZED SIMPLICITY
- Cartesian Corpuscular Philosophy
- Atom/Continuum

DYNAMICS
- Spatial and Temporal Hierarchy: Smith/Zener
- Nonequilibrium
- Path (History) Dependence
Cohen’s Reciprocity

Goal/means

Performance

Properties

Structure

Processing

Cause and effect
Hierarchy of Design Models

1. Quantum Design
   - SAM $K_{GB}(\Delta \gamma)$
2. Nano Design
   - SANS, XRD, APFIM, AEM
   - $\sigma_y$, H
   - LM, TEM

3. Micromechanics Design
   - $J_{IC}$, $\gamma_i$
   - LM, TEM, MQD, DSC

4. Transformation Design
   - FLAPW, DVM
   - RW-S

5. Solidification Design
   - DICTRA TC/$\Delta p_L$
   - TC/MART CASIS, MAP
   - ABAQUS/SPO TC, $\Delta V$
   - TC(Coh)/DICTRA ABAQUS/EFG
   - PrecipiCalc™
M2C Precipitation

M2C carbide precipitation behavior in AF1410 steel vs. tempering time at 510C following 1 hour solution treatment at 830C
Grain Boundary Embrittlement

Embrittlement Sensitivity
(K/at. %)

Example: Design Integration with CMD

Matrix + Strengthening Dispersion Design

Grain Pinning Dispersion Design

\[ \Delta G(M_2C)@482^\circ C \]

Peak VHN\( (482^\circ C) \)

Mo

\[ Ms(\circ C) \]

\[ Ts(\circ C) \]

2ppm, 5ppm, 10ppm

Austenitizing Temperature

Finish Forging Window

\[ Y(MX,Mo\#1) \]

\[ W(FCC,C) \]

\( (V,Mo)(C,N) \) Fraction
CyberSteels to Market

Ferrium C61          AMS6517

Ferrium S53 Stainless  AMS5922

Ferrium C64          AMS6509

Ferrium M54          AMS6516

T45

SCORE
INTERNATIONAL
OFF-ROAD RACING

A10

NASCAR

Questek Innovations LLC
n=701
n=129

Probability (Weibull scale)

Yield Strength, ksi

620°C
20°C

n=701
n=129
<table>
<thead>
<tr>
<th>Type</th>
<th>Tool</th>
<th>Company</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>Design integration</td>
<td>iSIGHT</td>
<td>Engineous Software (Salt Lake City, Utah)</td>
<td>Multidisciplinary design optimization (MDO)</td>
</tr>
<tr>
<td>CMD</td>
<td></td>
<td>QuesTek Innovations LLC (Evanston, Illinois)</td>
<td>Parametric materials design</td>
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<td>Macroscopic process modeling</td>
<td>ProCAST</td>
<td>ESI Group (Paris, France)</td>
<td>Solidification processing</td>
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<tr>
<td>CMD</td>
<td>DEFORM-HT</td>
<td>Scientific Forming Technologies Corporation (Columbus, Ohio)</td>
<td>Deformation processing and heat transfer (finite-element method)</td>
</tr>
<tr>
<td>Microstructural simulation</td>
<td>PrecipiCalc</td>
<td>QuesTek Innovations LLC (Evanston, Illinois)</td>
<td>High-fidelity precipitation simulation</td>
</tr>
<tr>
<td>CMD</td>
<td>DICTRA</td>
<td>ThermoCalc AB (Stockholm, Sweden)</td>
<td>Multicomponent diffusion</td>
</tr>
<tr>
<td>J MatPro</td>
<td></td>
<td>Thermotech Ltd. (Surrey, United Kingdom)</td>
<td>Phase relations and basic microstructural modeling</td>
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<tr>
<td>Thermodynamics</td>
<td>ThermoCalc</td>
<td>ThermoCalc AB (Stockholm, Sweden)</td>
<td>Multicomponent thermodynamics and phase diagrams</td>
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<tr>
<td>CMD</td>
<td>Pandat</td>
<td>CompuTherm LLC (Madison, Wisconsin)</td>
<td>Multicomponent thermodynamics and phase diagrams</td>
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<tr>
<td>CMD</td>
<td>FactSage</td>
<td>Thermfact CRCT (Montreal, Canada)</td>
<td>Multicomponent thermodynamics and phase diagrams</td>
</tr>
</tbody>
</table>
S53 System Flow-Block Diagram

**PROCESSING**
- Tempering
- Solution Treatment
- Hot Working
- Solidification
- Deoxidation
- Refining

**STRUCTURE**
- Matrix
  - Lath Martensite: \( M_S \geq 200^\circ C \)
  - Ni: Cleavage Resistance
  - Co: SRO Recovery Resistance
  - Cr: Corrosion Resistance
- Strengthening Dispersion
  - \((Cr,Mo,V,Fe)\)\(_2\)C
  - Avoid Fe\(_3\)C, M\(_6\)C, M\(_7\)C\(_3\), M\(_{23}\)C\(_6\)
- Passive Film Formation
  - Cr partitioning into oxide film
  - \( E_{pp} \) and \( l_{crit} \)
- Microsegregation
  - Cr, Mo, V
- Grain Refining Dispersion
  - \( \alpha \) + \( \gamma \)
  - Microvoid Nucleation Resistance
- Grain Boundary Chemistry
  - Cohesion Enhancement: B, Re
  - Impurity Gettering: La, Ce

**PROPERTIES**
- Strength
  - \( \sigma_{UTS} \geq 280 \) ksi
  - \( \sigma_{YS} \geq 230 \) ks
- Aqueous Corrosion Resistance
  - \( \geq 15-5PH \)
- Stress Corrosion Resistance
  - \( K_{ISC} \geq 30 \) ksi\( \sqrt{\text{in}} \)
- Fatigue Resistance
  - \( \geq 300\text{M} \)
- Core Toughness
  - \( K_{IC} \geq 50 \) ksi\( \sqrt{\text{in}} \)
S53 Robust Design Sensitivity Analysis

Compositional Variations (wt%, ±6σ):
C ± 0.01  Cr ± 0.2  Mo ± 0.1
W ± 0.1  Co ± 0.3  Ni ± 0.1
V ± 0.02

Variations of:
Structure — carbide solvus T_s, martensite T_m, precipitation control ΔG’s
Property — hardness HRC, toughness CVN

Results of 1000 runs (12 minutes on a Pentium IV 2.2GHz CPU)
Ferrium S53 — Design For Scale

Solidification Simulation

- S53-3 Segregation Experience
  - 300 lb 8” VAR ingot
  - Mag = 1500 X

Homogenization Simulation

- S53A Segregation Experience
  - 3000 lb 17” VAR ingot
  - Mag = 2000 X

Graphs showing the distribution of Mo, Co, Cr, Ni, Mo, W, C, and V over time and distance.
S53 AIM Analysis for UTS

AIM prediction

Heat 1
Heat 2
Heat 3

Experimental Data

Probability

UTS, ksi

AMS Specification
MMPDS A-Allowables

+3σ
-3σ
Mean value

Property
M54 AIM Analysis for UTS

AIM prediction

Heat 1
Heat 2
Heat 3

Probability

UTS, ksi

275 280 285 290 295 300 305
Computational Materials Qualification Acceleration

**TRL Milestones**
- **TRL7**: first landing gear field service test flight
- **TRL6**: system integration
- **TRL5-6**: first component rig test
- **TRL3-4**
- **TRL2**
- **TRL1**

**Material Development Milestones**
- MMPDS handbook update issued
- Additional property data developed
- 10th multi-ton full-scale ingot produced
- Aerospace Materials Spec. issued
- Static property data developed
- 3rd multi-ton full-scale ingot produced
- 1st multi-ton full-scale ingot produced
- Prototype static properties demonstrated
- Design goals established

Dates

- Jan-99
- Jan-00
- Jan-01
- Jan-02
- Jan-03
- Jan-04
- Jan-05
- Jan-06
- Jan-07
- Jan-08
- Jan-09
- Jan-10
- Jan-11
- Jan-12
- Jan-13
- Jan-14

5 design iterations

1 design iteration
Materials by Design
• Design Exploration and Optimization
• Robust Analysis
Tools: QuesTek CMD/MaDe, iSIGHT

Accelerated Insertion of Materials
• Probability-Based Variational Analysis and Data Development
Tools: QuesTek Proprietary Software, iSIGHT, JMP

Mechanistic Models
• Process-Structure Models
• Structure-Property Models
Tools: QuesTek Proprietary Software, PrecipiCalc, ThermoCalc, DICTRA, ABAQUS, DEFORM, etc.

Fundamental Material Databases
• Thermo-Chemical Data
• Physical Parameters
Tools: CALPHAD (ThermoCalc, DICTRA databases), First-principle (FLAPW, VASP), etc.
## ICME MS Program

<table>
<thead>
<tr>
<th>Required Core</th>
<th>F</th>
<th>W</th>
<th>S</th>
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<tbody>
<tr>
<td>MSc 401</td>
<td>Analytical &amp; Statistical Thermodynamics</td>
<td>MSc 408 Phase Transformations in</td>
<td>MSc 390 Materials Design</td>
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<tr>
<td>PSED 510-1</td>
<td>0.5 ICME Seminar</td>
<td>Materials</td>
<td>PSED 510-2 0.5 ICME Seminar</td>
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<td>MSc 391</td>
<td>Process Design</td>
<td>MSc/ESAM 495 Introduction to Statistical Mechanics</td>
<td>MSc 406 Mechanical Properties of Materials</td>
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<td>MSc/ESAM 495</td>
<td>Modeling of Soft Materials</td>
<td>ME/CCE 426-1 Computational Mechanics I</td>
<td>ME/CCE 426-2 Computational Mechanics II</td>
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<tr>
<td>CEE 327/ME 365</td>
<td>Introduction to FEM</td>
<td>ME 366 Finite Elements for Design &amp; Optimization</td>
<td>Phys 450 Advanced Computational Condensed Matter Physics</td>
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<table>
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<tr>
<th>Recommended Electives</th>
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<tbody>
<tr>
<td>ME 341</td>
<td>Computational Methods for Engineering Design (or ME 441 Engineering Optimization for Product Design &amp; Manufacturing)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
I. Civil Shield (EDC)  
Client: ONR, DHS, Trinity R  
Advisor: Dr. Zack Feinberg  
**Team:** Ma, Maethasith, Richardson, Schwenker, Zhao

II. Earthquake Steel  
Client: ArcelorMittal  
Advisor: George Fraley  
**Team:** Cool, Gross, Rawlings, Tran

III. FSW Joinable Aluminum  
Client: Boeing, Ford  
Advisor: Ricardo Komai  
**Team:** Brodnik, McGinnis, Pai, Ricks

IV. HP Magnesium  
Client: ARO, GM, DOE  
Advisor: Dr. Dennis Zhang  
**Team:** Han, Na, Park

V. TRIP Titanium  
Client: ONR  
Advisor: Jiayi Yan  
**Team:** Savoie, Wengrenovich

VI. HP Shape Memory Alloy (EDC)  
Client: Medtronic, GM  
Advisor: Dana Frankel  
**Team:** Jin, Kadleck, Poupard, Yoo
UHS Stainless Steels for Landing Gear

Accidents by Aircraft System
Commercial Jet Transport Aircraft
1958-1993

Source: FLIGHT SAFETY FOUNDATION-FLIGHT SAFETY DIGEST-DECEMBER 1994

**Issues:**
- Over $200M spent in LG per year
- 80% corrosion related SCC failures
- Cad plating used to protect current steel
- Known carcinogen (AF 2000 lb/yr)

**Stainless Benefits:**
- Dramatic reduction in LG cost (60% = $120M per year)
- Significant reduction in SCC failures
- Cadmium plating not required
- General corrosion mitigated
- 80% of Steel Condemnations Avoided
M54: NAVAIR SBIR program goals for LG steels

- Enhanced landing gear life
- Navy replacement for AMS 6532 (Aermet®100)
  - Equivalent-to-better properties
  - Tensile (including ductility)
  - Fracture toughness
  - SCC resistance
  - Significantly lower cost