COMPUTATIONAL MATERIALS DESIGN FOR ACCELERATED IMPLEMENTATION

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Northwestern University / QuesTek Innovations LLC
Evanston IL

DOE SC-NE Workshop on Advanced Computational Mat. Sci.
March 31, 2004
**MTL/SRG**

A) Cybersteel 2020: Ultratough Plate Steels (ONR; CAT)

B) HT Carburizing Steels (DOE-OIT; GM, P&W)

C) Superalloys (AF-MEANS, DARPA-AIM; RMCI)

D) Bulk Metallic Glasses (DARPA-SAM)

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PROCESSING

- TEMPERING
- SOLUTION TREATMENT
- HOT WORKING
- SOLIDIFICATION
- DEOXIDATION
- REFINING

STRUCTURE

- MATRIX
  - Lath Martensite
  - Ni: Cleavage Resistance
  - Co: SRO Recovery Resistance

- STRENGTHENING DISPERSION
  - (Mo, Cr, W, V, Fe)\(_2\)Cx
  - (Nb, V)Cx
  - Avoid Fe 3C, M6C, M23C6

- GRAIN REFINING DISPERSION
  - \(\frac{d}{f}\)
  - Microvoid Nucleation Resistance

- AUSTENITE DISPERSION
  - Stability (Size, Comp.)
  - Amount
  - Dilatation

- GRAIN BOUNDARY CHEMISTRY
  - Cohesion Enhancement
  - Impurity Gettering

PROPERTIES

- STRENGTH
- TOUGHNESS
- HYDROGEN RESISTANCE

PERFORMANCE
Transformation Design

Micromechanics Design

Nano Design

Quantum Design

Solidification Design

LM, TEM
MQD
DSC

LM, TEM
J_{IC}, \gamma_i

SANS, XRD
APFIM, AEM

\sigma_y, H

SAM
K_{GB}(\Delta\gamma)

LM
SEM/EDS

TC/MART
CASIS, MAP

TC(Coh)/DICTRA - K_C
ABAQUS/EFG

PPT-H

K_C

TC/\Delta\rho_L

TC, \Delta V

ABAQUS/SPO

TC, \Delta V

TC(Coh)/DICTRA - K_C

ABAQUS/EFG

FM
DVM

RW-S
S53 Nanostructured UHS Stainless Results

Fracture Toughness vs. Ultimate Tensile Strength

Typical Fracture Toughness $K_{IC, L-T}$ (KSI/IN$^{1/2}$)

Ultimate Tensile Strength (KSI)

- 15-5PH
- 13-8Mo
- Custom 465
- AF 1410
- AerMet 100
- Ferrium S53
- 4340/300M
Multiscale Ductile Fracture Simulator

Microvoiding matrix + primary particles

Iron matrix + secondary particles

Subatomic scale

Fracture toughness

CAT Steel

\( \sigma_Y = 1.1 \text{GPa} \)
\( d\sigma/d\varepsilon = 0.6 \text{ GPa} \)

\( \delta_{IC} = 120 \mu\text{m} \)
\( \gamma_i = 0.2 \)

\( f_{\text{TiN}} = 0.052\% \)
\( d_{\text{TiN}} = 1-10 \mu\text{m} \)

\( f_s = 0.015\% \)
\( d_s = 0.003-3 \mu\text{m} \)
Current Applications

Gears: NASCAR
- Successfully completed race with narrow gear design
- Moving forward with development

Ring & Pinion: SCORE
- Finished entire race with new design
- Production sets being made

Dog Rings and Camshafts: Currently in testing

For more info contact: C. Kuehmann or B. Tufts - QuesTek Innovations LLC - 847-328-5800
Heterogeneous Precipitation of Austenite on Copper Particles

Isoconcentration surface with 10% Ni threshold
Toughness - Strength Combination

Charpy V-notch Energy Absorption at 27°C (ft-lb) vs. Yield Strength (ksi)

- NUCu-60
- NUCu-100
- NU Bridge Steels
- HY-80
- HSLA-100
- HY-130
- HY-180
- Blastalloy160
- Co-Ni Steels
- AF1410
- AerMet100
ARCHITECTURE DESIGN

Integration Infrastructure
iSIGHT framework provided by Engineous Software

Core Utilities
3rd Party tools to extend iSIGHT’s integration capabilities

Analysis Components
Models provided by Pratt & Whitney, General Electric, Questek, and others. Integrated by Engineous into the DKB architecture via iSIGHT

* Distributed Resource Management

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**PrecipiCalc™ Timeline**

### Software/Hardware Improvement

- **1/01**: Birth
- **6/01**: Base Start
- **1/02**: Option Start
- **6/02**: PWA1100 F117 disk center
- **R88 coupons**

#### Lattice Parameters
- **γ/γ’**

#### Diffusivity Scaling
- 24 hours* on Pentium III 600MHz
- 2 hours* on Pentium III 1GHz with improved numerical nucleation treatment

#### Coherency Transition \(\sigma(R)\)
- 0.6 hours* on Pentium IV 2.2 GHz with compiler optimization
- 0.3 hours* on Pentium IV 2.2 GHz with optimized parameters
- 0.05 hours* on Pentium IV 2.2 GHz with cluster hardware

#### Applications/Demonstrations

- **1/03**: minidisk selected locations
- **iSIGHT integration with grain size and APB energy models**
- **spatial minidisk**
- **uncertainty error analysis**
- **prior heat treatment**
- **\(\gamma'/\text{carbide grain pinning}\)**

- **6/03**: R88 tensile samples
- **spatial V2500**

### Diffusivity Scaling

- **202x190**

### Coherency Transition

- **σ(R)**

### Applications

- **3D/2D mapping**
- **Option**
- **Start**
- **3D/2D**
- **3D/2D**

### Multiphase Interaction

- **minidisk**
- **spatial**

### Uncertainty Error Analysis

- **\(\gamma'/\text{carbide grain pinning}\)**

* single IN100 PWA1100 simulation
Composition Profile (at.%) across Matrix Channel in between Secondary Precipitates w. Tertiary Precipitate in IN100 - Center 1st Disc

- **Ni**: Diffusion field in Secondary $\gamma'$ precipitates
- **Al**: Secondary $\gamma'$ precipitates
- **Ti**: Tertiary $\gamma'$ precipitate (not fully resolved in this representation)
- **Co**: Tertiary $\gamma'$ precipitate (not fully resolved in this representation)
- **Cr**: $\gamma$ Matrix channel
- **Mo**: Secondary matrix inclusion within secondary $\gamma'$ precipitate (not fully resolved in this representation)

Dieter Isheim, 8Dec 2002
Northwestern University
Impact of DARPA AIM Initiative

• Supply chain impact on material capability captured

➢ Enables versatile processing for smaller lot sizes

Weibull probability paper

PrecipiCalc

YS model

Yield Strength

1150F, integral data, sample size = 701
RT, integral data, sample size = 129
1150F, simulation 110303, sample size = 377
RT, simulation 110303, sample size = 377

chemistry

yield strength, ksi

145 150 155 160 165 170 175
0.001 0.010 0.050 0.100 0.250 0.500 0.750 0.900 0.990
## Minidisk Microstructure Prediction with PrecipiCalc

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<th>Minidisk Comparison</th>
<th>Bore</th>
<th>Rim</th>
<th>Attachment</th>
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<td>Primary $\gamma'$</td>
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<tr>
<td>Fraction (%)</td>
<td>24</td>
<td>22.6</td>
<td>23.5</td>
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<tr>
<td>Size (µm)</td>
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<td>1.23</td>
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<td>Secondary $\gamma$</td>
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<td>Fraction (%)</td>
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<td>Size (nm)</td>
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<td>Tertiary $\gamma'$</td>
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<td>Size (nm)</td>
<td>18</td>
<td>21.5</td>
<td>19.7</td>
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### Diagram

- **Attachment**
- **Bore**
- **Rim**
Impact of DARPA AIM Initiative

- Material behavior intimately linked and participating in the design process
  - 4 months to improved capability
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 Ts, martensite Ms, precipitation control ΔG’s
- Property — hardness HRc, toughness CVN

Results of 1000 runs (12 minutes on a Pentium IV 2.2GHz CPU)
S53A Scale-up Properties

- **YS [ksi]**
  - S53A (300 pound heat): 63
  - S53A (3,000 pound heat): 60

- **UTS [ksi]**
  - S53A (300 pound heat): 285
  - S53A (3,000 pound heat): 285

- **El. [%]**
  - S53A (300 pound heat): 15
  - S53A (3,000 pound heat): 16

- **RA [%]**
  - S53A (300 pound heat): 59
  - S53A (3,000 pound heat): 63
Processing

- Coating
- Surface Treatment
- Aging
- Solution Treatment
- Solidification + Shaping
- Melt Refining

Structure

- Thermal Barrier Coating
- Oxygen Barrier Coating
- Bond Coat
- Oxide Scale (Al₂O₃, YAG)
- Film Interface

Properties

- Oxidation Resistance
  - Higher Dₐ/Dₒ
  - Low Oxygen Solubility

- Creep Strength
  - Dispersion Stability

- Ductility/Embrittlement Resistance
  - Metallic Matrix (with low O₂ solubility)

Solid Solution

- Lattice Parameters
- Solid Solution Strengthening
- Oxygen Activity
- Control Diffusivities

Dispersed Phases: PdAl,YAl (Pd,Pt, Ru)₂(Hf,Zr,Y,Nb)Al

- Lattice misfit
- High Stability
- Coherent Interface
- Low Coarsening Rate Constant
Tie-tetrahedra in the Nb-Pd-Hf-Al quaternary system at 1200°C
Relative Charge in Octahedral Hole versus Metal Substitutional
Diffusivity of Al in a Nb-X-5Al (in at%) bcc solid solution

Diffusivity of Al (m^2/sec)

1300°C

mol fraction X (X=Hf,Ti,Cr)

10^{-14}

10^{-15}

10^{-16}
Oxide scale in Alloy A’ oxidized at 1300°C

A: \( \text{Al}_2\text{O}_3 + \text{HfO}_2 \)
B: \( \text{HfO}_2 \)
I. Blastalloy II: LC160 Martensite
   Client: ONR, Dr. Julie Christodoulou
   Advisors: Arup Saha; Yana Qian
   Team: Dan Cogswell, Joe Dudas, Ken Liu

II. Blastalloy III: PH-TRIP Austenite
    Client: ONR, Dr. Julie Christodoulou
    Advisors: Dr. Su Hao; Zhe Liu
    Team: Danijel Gostovic, Sai-Pong Leung, Derek Norton

III. Dragonslayer II: Carburizing Stainless Bearing Steel (CS62+)
     Client: DOE-OIT, P&W, QuesTek
     Advisors: Dr. Jay Gao; Ben Tiemens
     Team: Loren Darling, Thor Gudmundsson

IV. MX4: Ni Aeroturbine Blade Alloy
     Client: NSF-FRG (OSU), P&W, GEAE
     Advisors: Dr. Gautam Ghosh; Chandler Becker
     Team: Travis Harper, Mike McCarren, Paul Von Donnen

V. Noburnium: Nb Superalloy
     Client: AF-MEANS, Dr. Craig Hartley
     Advisors: Abhijeet Misra; Dave Bryan
     Team: Erhan Altinoglu, Jennifer Bolos, Nora Colligan

VI. Terminator 4: FrankenSteel Goes to Mars (Biomimetic Self-Healing Alloy Composite)
     Client: NASA-Houston, Dr. Brad Files
     Advisors: Jin-won Jung; Michele Manuel
     Team: Wendy Cheng, Steve Knapp, Richard Scheunemann

VII. HT Aluminum/Bulk Metallic Glass
     Client: DARPA-SAM, Boeing, P&W, QuesTek
     Advisors: Ryan Rathbun; Keith Knipling
     Team: Bryan Harder, Nik Hrabe, Alison Markowitz
V-Cr-Ti Alloys

Isothermal Section at 600°C

Solubility Limits of C and O in V-4.1Cr-4.3Ti at 1000°C
Paradigm Shifts: MSE Integration

a) discovery based → design based
   - downstream cost of discovery

b) empirical → mechanistic/predictive

c) statistical (eng.)
   deterministic (sci.)
   } → probabilistic
   - prediction of multiple properties from defect distribution functions
   - designed variation (predictive robust design: performance/variation tradeoff)

d) computational mat. sci. (toys) → computational mat. eng. (tools)

e) reductionist analytical → holistic (systems) synthetic

Optimal Integration:
Tactical science in support of strategic engineering