A ROADMAP FOR VIRTUAL TESTING AND VIRTUAL PROCESSING OF CAST METALLIC MATERIALS

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1. MOTIVATION
   - Integrated Computational Materials Engineering
   - Virtual design of cast metallic components

2. Virtual processing of Ni-based superalloys

3. Virtual testing of Ni-based superalloys

4. Conclusions
Objective

Virtual design, virtual processing and virtual testing of new materials *in silico*, before they are actually manufactured in the laboratory.

Benefits

Accelerate materials development (reduce time to market).
Integrate materials into the design optimization process.
Unify design and manufacturing.

Strategy

Integration of all available modeling tools into a multiscale strategy capable of simulating processing, structure, properties and performance of engineering materials.

What is the worst scenario for ICME?

cast Al alloys (J. E. Allison, JOM, 2006)

Mechanical properties of cast metals (stiffness, strength, toughness, fatigue limit) depend on phenomena and structures that span over 9 orders of magnitude!
Virtual design of cast metallic components

VIRTUAL DESIGN

VIRTUAL TESTING

VIRTUAL PROCESSING

CFD

Porosity & defects
Residual stresses
Temperature distribution

Phase field

Phases
Driving force
Gibbs energy

Mobilities, Interfacial energy, Growth rate

Computational thermodynamics

Heat Capacity
Enthalpy, Crystal structure

MD/MC

Computational kinetics

Atomic/interface mobility
Lattice information
Elastic constants

MD/KMC

Continuum Mechanics

Polycrystal deformation
Texture evolution

Polycrystal homogenization

Single crystal plasticity model

DD

Macroscopic deformation and failure

Microstructure

European Research Council
Established by the European Commission

Supporting top researchers from anywhere in the world
VIRTUAL CASTING OF ENGINEERING ALLOYS

Component design

Porosity
Grain size

Mold filling & solidification simulation

Geometry

Solidification

Validation

Thermal

computational thermodynamics

Casting experiments

component & wrapping
MAR 247 is a polycrystalline Ni-based superalloy with outstanding mechanical properties at high temperature due to the W, Hf and Ta content, which is widely used in nozzle guide vanes, blades and disks in gas turbines.

### Chemical composition

<table>
<thead>
<tr>
<th>Element</th>
<th>Ni</th>
<th>W</th>
<th>Cr</th>
<th>Mo</th>
<th>Co</th>
<th>Al</th>
<th>Ti</th>
<th>C</th>
<th>Hf</th>
<th>Ta</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weight (%)</td>
<td>balance</td>
<td>10</td>
<td>8.4</td>
<td>0.7</td>
<td>10</td>
<td>5.5</td>
<td>1.05</td>
<td>0.15</td>
<td>1.4</td>
<td>3.1</td>
</tr>
</tbody>
</table>

### COMPONENT

Nozzle guide vane for a gas turbine with complex shape and thinner wall sections to be manufactured by investment casting designed by ITP.

Accurate prediction of the temperature profile in the cast during solidification is critical. This is a very difficult task because of the different heat transfer mechanisms (radiation, conduction, convection) and the different materials involved (metal, mould shell and insulation wrap), together with the corresponding interfaces.
Finite element model of the NGV, mould and wrapping.
The thermal properties of the different materials and interfaces were fitted from the experimental temperatures measured in the casting experiments.
Shrinkage porosity and microporosity were computed by taking into account the progress of solid, mushy and liquid regions in the cast during solidification.

Grain size and shape was determined by means of a Cellular Automata model that assumed grain nucleation on the mould surface.

The nucleation rate was given by
\[
\frac{dn}{d(\Delta T)} = \frac{n_{\text{max}}}{\sigma_{\Delta T} \cdot \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\Delta T - \Delta T_m}{\sigma_{\Delta T}} \right)^2 \right]
\]
where \( \Delta T \) was the local undercooling and \( n_{\text{max}}, \Delta T_m \) and \( \sigma_{\Delta T} \) are the model parameters.

Grain orientation was random and grain growth was given by
\[
v(\Delta T) = a\Delta T^2 + b\Delta T^3
\]
**GRAIN SIZE in a GUIDE VANE**


<table>
<thead>
<tr>
<th></th>
<th>Leading edge</th>
<th>Middlepart</th>
<th>Trailing edge</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Grain size (µm)</strong></td>
<td>1560</td>
<td>785</td>
<td>281</td>
</tr>
<tr>
<td><strong>Exp.</strong></td>
<td>1345</td>
<td>869</td>
<td>397</td>
</tr>
<tr>
<td><strong>Std. deviation</strong></td>
<td>813</td>
<td>451</td>
<td>213</td>
</tr>
<tr>
<td><strong>Exp.</strong></td>
<td>508</td>
<td>361</td>
<td>138</td>
</tr>
<tr>
<td><strong>Aspect ratio</strong></td>
<td>2.2</td>
<td>2.5</td>
<td>1.6</td>
</tr>
<tr>
<td><strong>Exp.</strong></td>
<td>2.5</td>
<td>3.0</td>
<td>2.0</td>
</tr>
<tr>
<td><strong>Model</strong></td>
<td>2.5</td>
<td>3.0</td>
<td>2.0</td>
</tr>
</tbody>
</table>

[Details on the table and images]
Virtual testing of polycrystalline materials can now be achieved by means of computational homogenization.

**Key ingredients**

**Microstructural features**: Grain size, shape and orientation distributions *easily* obtained by means of 2D and 3D characterization techniques (including serial sectioning, X-ray μtomography, 3D EBSD, X-ray diffraction, etc.)

**Single crystal behavior**: CRSS for each slip system and twinning (including latent and forest hardening) provided by
- Multiscale modelling
- Mechanical tests of single crystals
- Inverse problem: back up single crystal behavior from tests on polycrystals
  * Homogenization of polycrystals
  * Nanoindentation
polycrystalline IN718

single crystal properties (T, strain rate) from micropillar tests

Macroscopic mechanical properties (strength, fatigue, creep)

single crystal plasticity model

Inconel 718 is a polycrystalline Ni-based superalloy used in cast or wrought form for high temperature structural applications up to 650-700°C. The most widely used Ni-based superalloy due to its good castability and weldability, high mechanical properties and corrosion resistance and low cost.

**Chemical composition**

<table>
<thead>
<tr>
<th>Element</th>
<th>Ni</th>
<th>Fe</th>
<th>Cr</th>
<th>Mo</th>
<th>Nb</th>
<th>Al</th>
<th>Ti</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weight (%)</td>
<td>balance</td>
<td>18.5</td>
<td>19.0</td>
<td>3.0</td>
<td>5.1</td>
<td>0.5</td>
<td>0.9</td>
<td>0.04</td>
</tr>
</tbody>
</table>
Single crystal properties as a function of orientation, temperature and strain rate were obtained by means of micropillar compression tests.
Micropillar compression tests show limited experimental scatter. Partial unloadings were due to dislocation bursts.
No size effects on the initial CRSS nor in the strain hardening were observed for micropillars with $D > 3 \, \mu m$.

This is very likely due to the fact that the strength is controlled by the small spacing between $\gamma'$ and $\gamma''$ precipitates.
The CRSS were obtained by fitting the micropillar compression tests with numerical simulations carried out using a crystal plasticity finite element model.

A crystal plasticity model was implemented as a UMAT in Abaqus/Standard

Multiplicative decomposition $F = F^e F^p$ ; velocity gradient $L = L^e + F^e L^p F^{-1}$

Plastic deformation in a FCC crystal is accommodated by $N (=12)$ slips systems corresponding to the $\{111\}(110)$ family:

$$L^P = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha (S^\alpha \otimes m^\alpha)$$

The Green-Lagrange elastic strain is expressed as $E^e = \frac{1}{2} (F^e^T F^e - I)$

and the second Piola-Kirchoff stress tensor is given by

$$S = CE^e = C \left[ \frac{1}{2} \left( F^e^T F^e - I \right) \right]$$

where $C$ stands for the fourth-rank elastic stiffness tensor of the crystal.
The single crystal behaves as an elasto-viscoplastic solid:

- Shear strain rate in system $\alpha$: 
  \[ \dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{\tau_c^\alpha} \right|^{1/m} \text{sgn}(\tau^\alpha) \]

- Resolved shear stress in system $\alpha$: 
  \[ \tau^\alpha = C \left[ \frac{1}{2} \left( F_e^T F_e - I \right) \right] : (s^\alpha \otimes m^\alpha) \]

- Critical resolved shear stress in system $\alpha$: 
  \[ \tau_c^\alpha = \sum_{\beta} q_{\alpha\beta} h \left| \dot{\gamma}^\beta \right| \]

- Hardening modulus $h$ is given by the Voce Model:
  \[ h(\gamma) = h_s + (h_0 - h_s + \frac{h_0 h_s \gamma}{\tau_s - \tau_0}) \exp \frac{-\gamma h_0}{\tau_s - \tau_0} \]
  \[ \gamma = \int_0^t \sum_{\alpha} \left| \dot{\gamma}^\alpha \right| dt \]

The mechanical behavior of the single crystal is given by:

- $C_{11} = 260$ GPa; $C_{12} = 179$ GPa; $C_{44} = 110$ GPa for IN718
- $\tau_0$, $\tau_s$, $h_0$, $h_s$, $q_{\alpha\beta}$ and the strain rate sensitivity $m$ are obtained from micropillar compression tests.
Limited strain rate sensitivity of IN718 at ambient temperature.
Micropillar compression tests were simulated using the crystal plasticity model. The model includes the curvature at the fillet and the taper angle ($\approx 1.5^\circ$). The flat punch was modelled as rigid body with a lateral stiffness of 10 $\mu$N/nm. Coulomb friction ($\mu = 0.1$) between flat punch and micropillar. Discretization with 8-noded liner brick elements (C3D8).
PARAMETER IDENTIFICATION CRYSTAL PLASTICITY MODEL

<table>
<thead>
<tr>
<th>$\tau_0$ (MPa)</th>
<th>$\tau_s$ (MPa)</th>
<th>$h_0$ (GPa)</th>
<th>$h_s$ (GPa)</th>
<th>$q_{\alpha\beta}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>466</td>
<td>599</td>
<td>6</td>
<td>0.3</td>
<td>1</td>
</tr>
</tbody>
</table>

Effect of strain rate (single slip $<123>$ and $<235>$)

(a) $5 \mu m$

(b) $5 \mu m$

![Graphs showing the effect of strain rate on CRSS and plastic strain for experiment and simulation.](image)
Effect of double slip: coplanar $<414>$ and non coplanar $<012>$

![Graph showing CRSS vs Plastic strain for different slip systems with experimental and simulation data.]

Table:

<table>
<thead>
<tr>
<th>Slip System</th>
<th>CRSS (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(111)[-101]</td>
<td>0.49</td>
</tr>
<tr>
<td>(-111)[101]</td>
<td>0.49</td>
</tr>
<tr>
<td>(1-11)[011]</td>
<td>0.43</td>
</tr>
<tr>
<td>(1-11)[110]</td>
<td>0.43</td>
</tr>
</tbody>
</table>

![Images showing microstructures at 4 and 5 µm scale for different slip systems.]

PARAMETER IDENTIFICATION CP MODEL
VALIDATION OF CRYSTAL PLASTICITY MODEL

Multiple slip condition \textless 001\textgreater 

![Graph showing compressive stress vs. plastic strain for experiment and simulation in the condition \textless 001\textgreater.](image)

![SEM image showing a crystal structure with a scale of 2 \textmu m.](image)
Deformed micropillar along <212>
The mechanical behavior of the polycrystal is computed by means of the finite element simulation of the mechanical behavior of a representative volume element of the microstructure with periodic boundary conditions.

**Representative Volume Element**

2D grain size distribution obtained from micrographs is transformed into 3D using **strip-star** (Basel University).

RVE is obtained by the Laguerre tessellation of an initial set of points obtained from a Monte Carlo algorithm to provide the actual grain size distribution 3D.

The orientation of the grains within the RVE was random.

**Average grain size**

\[ 90 \pm 52 \, \mu m \]
Discretization was carried out 10-noded quadratic tetrahedral elements (C3D10).

Sensitivity analysis: number of grains in RVE and number of elements per grain

The displacement of opposite pairs of nodes on the RVE surfaces $x_B - x_A = L_{AB}$ is given by $u_B - u_A = (F - I) L_{AB}$ where $L_{AB} = (L, 0, 0), (0, L, 0)$ or $(0, 0, L)$
Good agreement between experiments and simulations: validation of the strategy.
Opens the way for further developments: high temperature, fatigue, creep, etc…
Virtual design, virtual processing and virtual testing of engineering alloys is becoming feasible by means of multiscale, bottom-up approaches.

Current available approaches still have to rely in phenomenological models (cellular automata model of grain nucleation and growth) and experiments (micropillar compression) provide accurate predictions for engineering alloys components. That will be gradually replaced by rigorous models based on ab initio and atomistic simulations as well as by more sophisticated coupling between simulations tools (phase field - computational thermodynamics - computational kinetics).

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