Feature extraction and stereological characterisation of single crystal solidification structure

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IMPaCT Research Centre
Introduce the jet-engine and the high pressure turbine (HPT) blade

Understand HPT manufacture and most important material property

Introduce a new method for single crystal feature extraction and one for characterisation
Single-Crystal Dendritic Microstructure

Primary arm spacing
200 - 500 \( \mu m \)

Tip radius

Tertiary branch

Secondary arm spacing

PDAS

[001]
Directional Solidification

1. Chill Plate
2. Chill Ring
3. Baffle
4. Holding Coil
5. Melting Coil
6. Samples

- SMELTING ZONE
- HEATING ZONE (LIQUID)
- TRANSITION ZONE (MUSHY)
- COOLING ZONE (SOLID)

WITHDRAWAL DIRECTION
First **remove** grain boundaries to improve the **creep performance**

A single-crystal material with a **refined** microstructure well **aligned** with [001] has superior creep resistance

But how can we **visualise** the microstructure??
(1) Feature extraction

(2) Stereological Characterisation
(1) Feature extraction

Before we can characterise single crystal microstructure we must extract the features (dendrite cores)
BSE Imaging of the Superalloy

$\phi = 9.4 \, mm$

Primary spacing calculated as a global constant via manual counting

Primary Spacing
Motivation and challenges

• Images are very noisy

• Multiple bright and dark areas

• Dendrites are highly random

• Contrast difference between features is small
Algorithm for automatic recognition of dendritic solidification structures

3 main stages

DenMap is **fully automatic**

For full explanation of the DenMap feature extraction algorithm please see:

Stage 1: Image filtering

- Black spots, stripes, contrast invariance disrupt the algorithm, reducing effectiveness

- 3 stages in the filtering to create a robust algorithm

\[ A \rightarrow B \rightarrow C \rightarrow D \]

Processing steps SEM image (CMSX-4)
Stage 1: Image filtering

A->B) FFT band pass filter (FFTBPF)

- Supresses small features
- Normalises the contrast
- Greatly improves the binarisation of the image

A) Original image

B) FFTBPF result
Stage 1: Image filtering

B->C) Histogram equalisation

- Sharpens the image and adjust brightness

C->D) Noise removal

- Smooth the intensity profile via extrapolation
• Rotation must be known to perform pattern recognition (NCC)

Rotation calculation by fitting rectangle for the maximum length in y-axis by rotating between $-22.5^\circ$ to $+22.5^\circ$

Stage 2: Generate Template

$Height = 5.46 \text{ cm}$

$Height = 5.76 \text{ cm}$

$Height = 5.9 \text{ cm}$

$=>maximum$
Scale must also be known

- A contour algorithm is used to detect dendritic shapes
- Strict selection is applied to acquire only clearly defined shapes
- The shape is scanned across with thickness calculated

Example image of a dendrite detected by a contour algorithm.

The thickness of the dendrite from left to right
Stage 3: Mapping

Normalised cross correlation (NCC)

- Scan a Template over an SEM Image row by row

Template scanning procedure

Similarity value for each pixel
Stage 3: Mapping

How to obtain the cores?

1. NCC output
2. Calculate threshold
3. Apply threshold

Statistical analysis between NCC and nearest neighbour distances of detected cores

Original image
NCC output
Threshold output
Map into a binary image
Calculate centroids
The Result

<table>
<thead>
<tr>
<th>Sign</th>
<th>In words</th>
<th>Meaning</th>
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</thead>
<tbody>
<tr>
<td>+</td>
<td>Red crosses</td>
<td>Identified cores</td>
</tr>
<tr>
<td>○</td>
<td>Green circles</td>
<td>Manually selected</td>
</tr>
<tr>
<td>○</td>
<td>Blue circles</td>
<td>Missed out cores</td>
</tr>
<tr>
<td>○</td>
<td>Purple circles</td>
<td>Similar shape and intensity to a dendrite core but smaller</td>
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</table>

- Image size: 8947x9271 pixels,
- Accuracy: 98.4%,
- Time: 89 s

Mapped image
DenMap Automatic Dendrite Detection

508 dendrites

∅ = 9.4 mm

55 seconds

FASTER THAN COUNTING!
(2) Stereological Characterisation

We have the features now we must develop a method to determine the nearest interacting neighbours for each dendrite within the bulk array.
1st perform Voronoi Tessellation of the dendritic array to separate the bulk image into local regions.

$\phi = 9.4 \text{ mm}$
We develop a method to characterise the single crystal that uses local packing patterns. We look at individual dendrites within the bulk array and in effect ask the question ‘what packing best characterises this local neighbourhood’. We characterise local packing around each dendrite from triangular (N3) to nonagonal (N9) (see table below).

<table>
<thead>
<tr>
<th>Coordination Number (N)</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
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<tbody>
<tr>
<td>Ideal Packing Arrangement</td>
<td><img src="image.png" alt="Diagram" /></td>
<td><img src="image.png" alt="Diagram" /></td>
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\[a \text{ \ is \ the \ side \ length \ which \ is \ fixed \ between \ outside \ neighbours.} \ \lambda_1 \text{ \ is \ the \ primary \ spacing (see \ slide \ 4 \ for \ definition)}\]
Distance-based Nearest Neighbours

Next the locally interacting neighbourhood must be determined. In the example below, Voronoi tessellation has determined the local arrangement to be nonagonal (a), however, our method calculates the real interacting neighbourhood to be closer to hexagonal (f).

For more detailed information on the method please see:

The bulk array is colour coded depending on the determined packing patterns. For example, the green regions correspond to hexagonally packed local arrangements (N6), whereas the dark purple indicate triangular packing (N3). The colour code is indicated below.

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<td>Ideal Packing Arrangement</td>
<td>( a \sqrt{\lambda_1} )</td>
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![Diagram showing packing patterns](image)
Once the local interacting neighbourhood is determined, the relationship between the local average distance between nearest neighbour (NN) dendrites to the central dendrite (local primary spacing - $\bar{\lambda}_{Local}$) and the coordination number ($N$) can be determined (see slide 23 for definition of $N$). Calculated as follows:

$$\bar{\lambda}_{Local} = \frac{\sum_{j=1}^{N} \sqrt{(x_j-x_0)^2 + (y_j-y_0)^2}}{N}$$

where, $x_0$ and $y_0$ indicate the coordinates of a core of interest; $x_j$ and $y_j$ are the coordinates of the NN around the core of interest; $j$ is an index that iterates from 1 to the number of identified NN.
Local Primary Spacing Versus Nearest Neighbours

The quantity of each type of packing (N) and the distribution of local primary spacing can now be determined across the array.
Local Primary Spacing versus Packing

Clear relationship between packing variation and local primary spacing distribution

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<tr>
<td>λ₁</td>
<td>1.7321</td>
<td>1.4142</td>
<td>1.1756</td>
<td>1.0000</td>
<td>0.8678</td>
<td>0.7654</td>
<td>0.6840</td>
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<tr>
<td>Kicients</td>
<td>1.5196</td>
<td>1.4142</td>
<td>1.4501</td>
<td>1.5197</td>
<td>1.5993</td>
<td>1.6817</td>
<td>1.7640</td>
</tr>
<tr>
<td>−3σ</td>
<td>−2σ</td>
<td>−σ</td>
<td>λ_{Array}</td>
<td>+σ</td>
<td>+2σ</td>
<td>+3σ</td>
<td></td>
</tr>
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BSE image of CMSX4 with 508 dendrites

Fully automatic centre detection 99% accuracy

Fully automatic characterisation

\( \phi = 9.4 \, mm \)

1 minute 25 seconds

FASTER THAN COUNTING!
Summary

➢ Fully automatic feature extraction and characterisation in 1 minute and 25 seconds

➢ New relationships between packing patterns and local primary spacing

➢ Refining local primary spacing will reduce distribution of inhomogenities and improve mechanical performance
Thank you