Intergranular Crack Propagation in Polycrystalline Metals

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Contents

• Background
• Creating model polycrystals
• Application of a model
• Experimental example
• Concluding remarks
Background 1- Brittle Fracture

- can occur in metals and alloys
- In some cases is associated with the well-established ductile-to-brittle transition temperature
- which is influenced by various factors during service, including thermal history and neutron irradiation, which can lead to grain boundary segregation and embrittlement.
- Modelling can help to improve the understanding of how brittle cracks initiate and propagate in polycrystalline materials.
- Various models have been developed to describe brittle fracture.
Background 2 – Brittle Fracture

EN1A Ferritic Steel

Intergranular Fracture

Transgranular Cleavage
Background 3

Modelling over different scales

![Graph showing different scales and times for modeling](image)
Creating Models 1

Model Characteristics
These are designed to ensure they obey mathematical relationships and match the size distributions of the model material

Geometrical Properties
- Precise structural information provides accurate values for areas and orientations of grain boundaries and cleavage planes
- Irregularly shaped 3D model grains can be compared with observations of specimens
- Differently sized grains
- Planar or curved faces depending on the growth law

Physical Properties
- Ability to assign crystallographic orientation for each grain (randomly or textured)
- Cleavage planes and fracture energies are determined by the model material
- Grain boundaries may be intact, cavitated, decohered, contain precipitates etc.
Creating Models 2

Steps required to create a three-dimensional model with polyhedral grains

• define the dimensions of the model
• position grain nuclei in model space (randomly or controlled)
• grow grains outward from nuclei until they meet neighbours and fill the model space
• extract the co-ordinates of vertices and identify edges, faces and relationships
• apply physical properties
Creating Models 3

Grain nuclei grow to fill cubic model space with parent voxels.

Voxels show grain connections.

Faces, edges and vertices determine grain shapes.

Stress
Brittle Fracture

- In general, there is competition between grain boundary fracture and fracture along cleavage planes. The choice is influenced by the number of cleavage planes for the model material and the relative fracture energy for each mode.
- Grain boundaries in the model may have different fracture strengths reflecting the thermo-mechanical history of the material.
- The easiest crack path also depends on the orientation of the possible fracture planes relative to the stress axis.
- At the edge of each new fracture facet, the software assesses each forward route and selects the weakest.
Fracture solely on grain boundaries is typical of a thermally or irradiation embrittled steel. Viewed from above the fracture surface is continuous.

Viewing from the side, shows the depth of the fracture path. There are fewer choices than when propagating by cleavage fracture and this creates a rougher fracture surface.
Application of Model 2

Fracture Surface

Fracture occurs on a well-oriented grain boundary and spreads outwards.

The crack propagates into each unfractured grain it meets, choosing the better oriented of the 2 faces ahead.

As more facets are added the crack becomes more jagged.

The perspective view of the first crack facet and its immediate neighbours
Application of Model 3

Faceted Fracture Surface

Eventually the crack crosses the model. This is not a sufficient condition for the model to separate as there may be dovetailing between the two parts.
**Experimental Example**

**Polycrystalline nickel**

<table>
<thead>
<tr>
<th>Chemical composition (wt%)</th>
</tr>
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<tbody>
<tr>
<td>Cu</td>
</tr>
<tr>
<td>0.01</td>
</tr>
</tbody>
</table>

- Solution heat treatment at 1017°C for 30min and air cooled
- Grain size 200 μm
- Three point bend geometry specimen with a notch (a/w = 1/3)
- The specimens tested in the temperature range -196°C to 200°C
- Brittle fracture along weak grain boundaries up to temperatures of 150°C
Intergranular fracture at room temperature (~20°C)

Limited ductility

EBSD grain orientation mapping

300 µm

500 µm
Experimental Example

brittle to ductile transition
Concluding Remarks

In modelling fracture, it is important to use three dimensional models.

Developing these realistic models of fracture in polycrystals has benefited from close collaboration between theorists and experimentalists.

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Perspective view of model crack