INTERACTIVE SESSION V: INITEAC TRAINING SESSION

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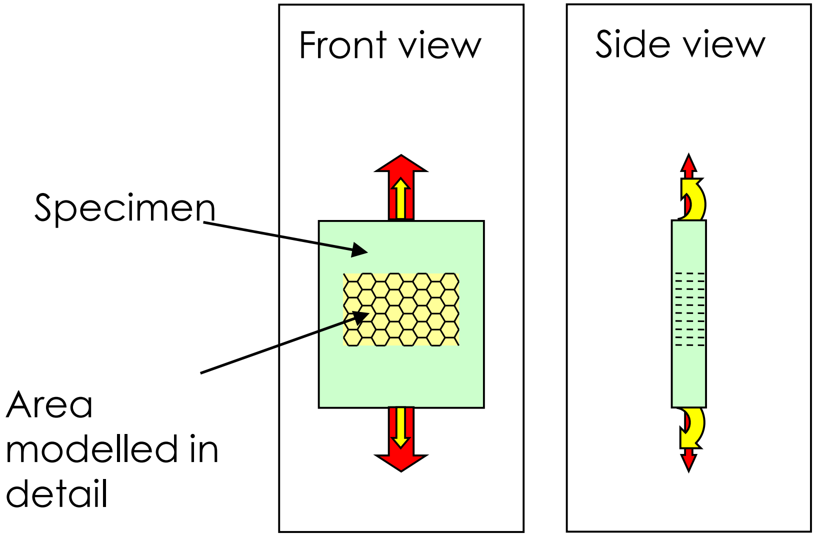
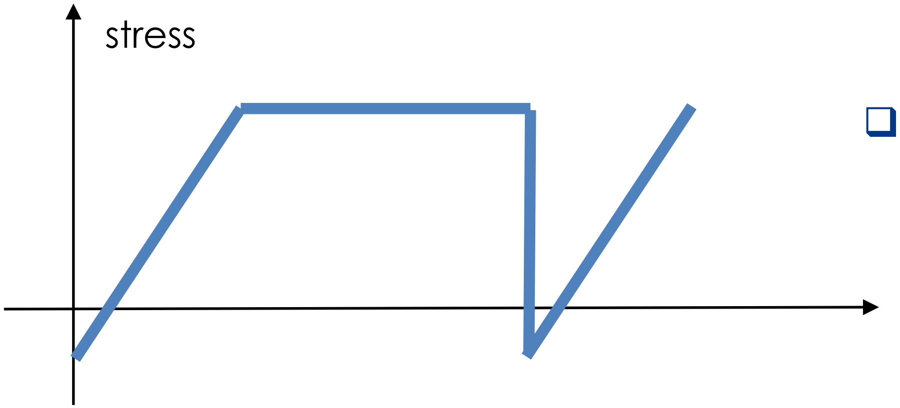
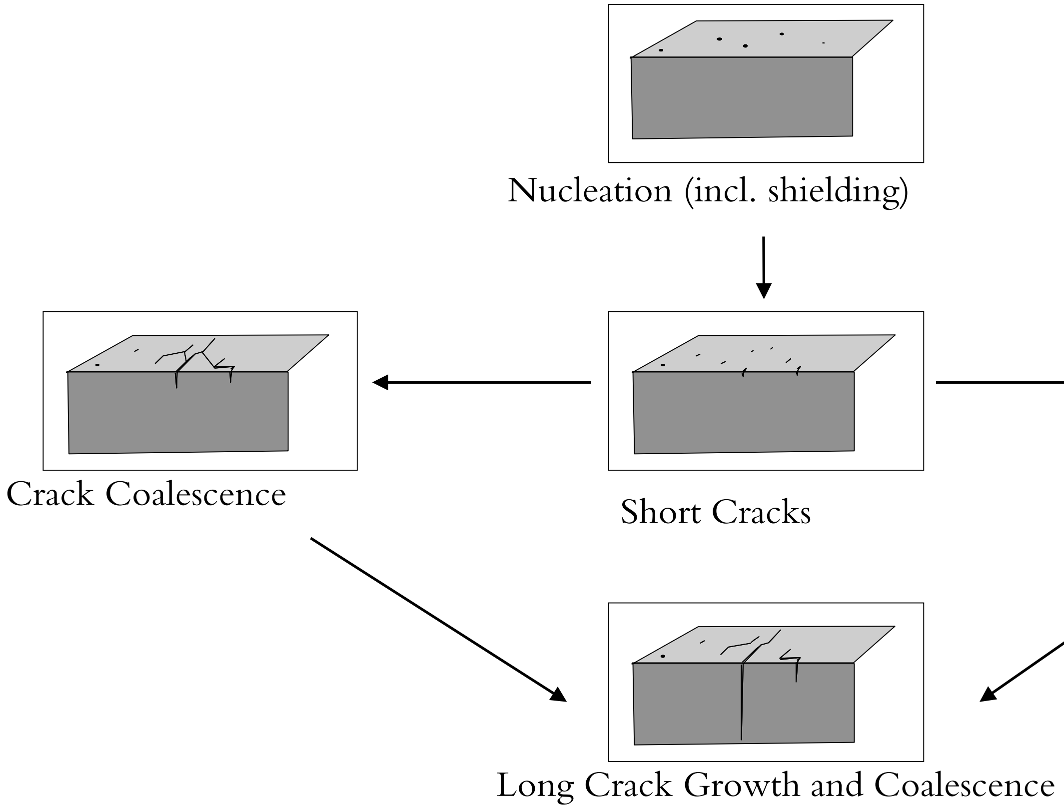
INITEAC: Overview





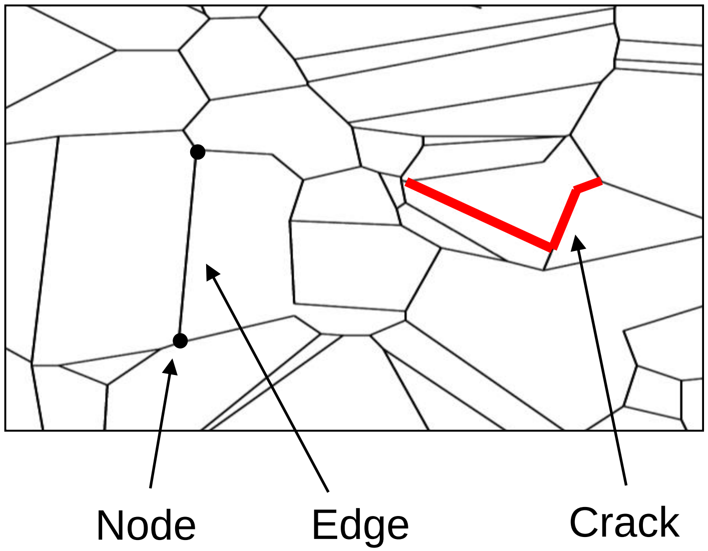
- Statistical modelling of IASCC
- Intergranular cracks only
- Based on 2D-map of grain boundaries at specimen surface
- Input: time profile of stress
- Output: histogram of crack lengths, crack ‘patterns’
- 2.5 D: statistical representation of 3rd dim. of grain structure. Properties of boundaries vary as growing into the depth.
- To run INITEAC need:
  - Input file (with control parameters)
  - Mesh file

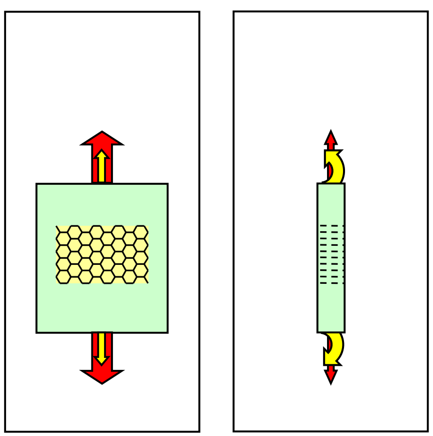
INITEAC: Overview



Different models for growth of small and long cracks

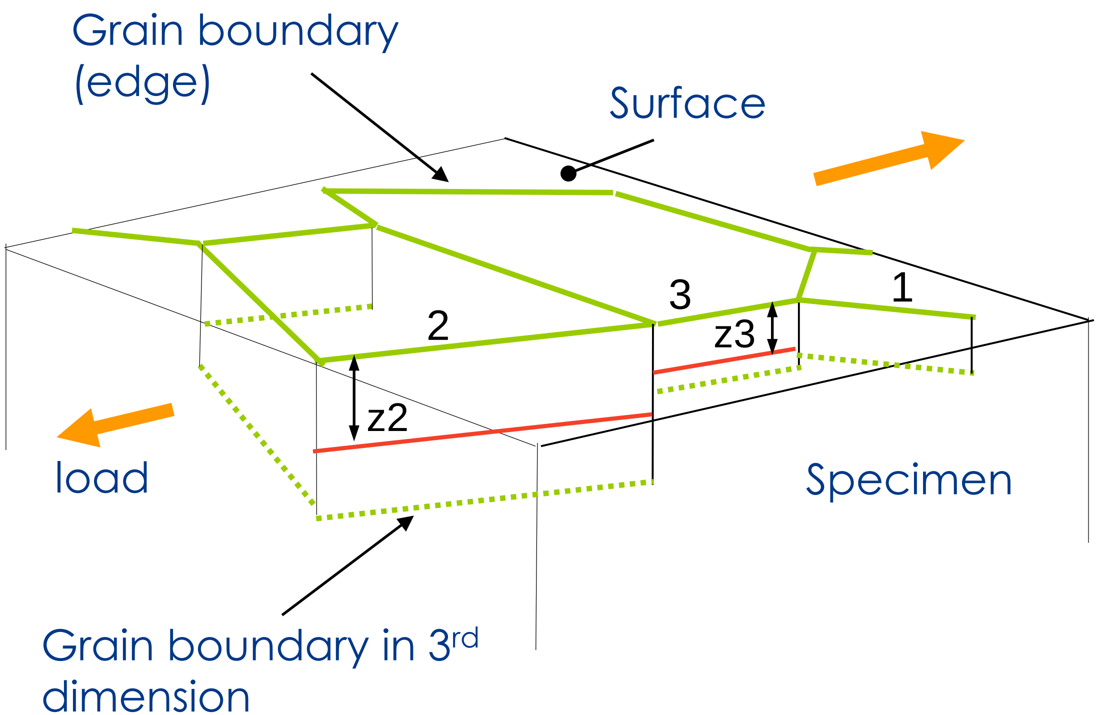
The mesh





- Import of arbitrary 2D grain map (nodes & edges)
- Each grain boundary (edge) is straight line between 2 nodes
- Each edge can be assigned properties, e.g. difference of orientation of adjacent grains
- <u>Code only deals with boundaries, not with grains</u>
- Cracks grow along surface (on grain boundaries) and into depth
- Short crack = set of adjacent edges with cracks growing deeper through damage development
- Long crack = growing according to fracture mechanics. Crack ends move along edges.

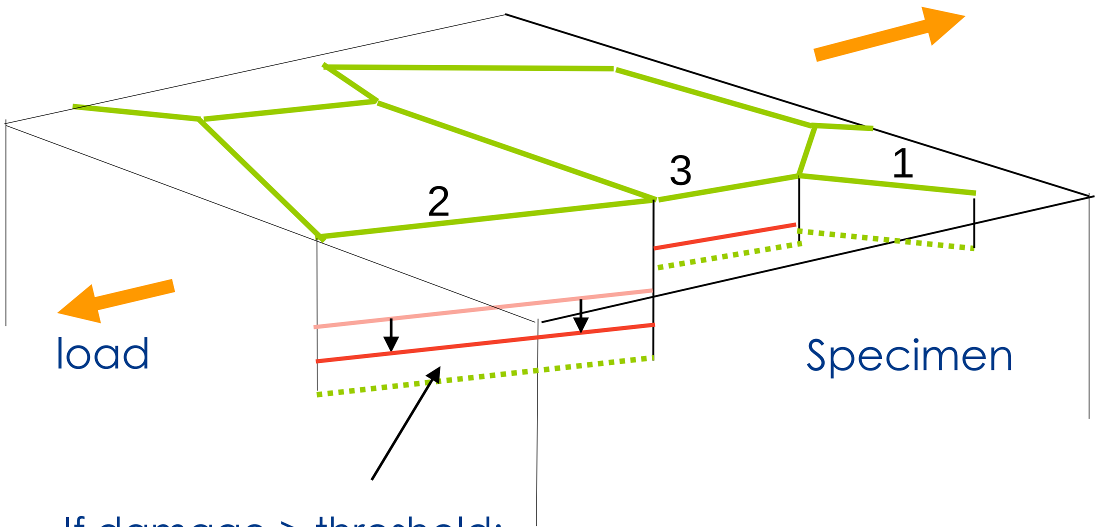
The mesh contd.



Each edge has:

- Boundary in 3rd dim.
- Depth, z (how far opened from surface)
- Damage (degree of oxidation/slip development)
- Sensitivity for rupture
- Properties (misorientation, Si, Cr, …) that determine Sensitivity

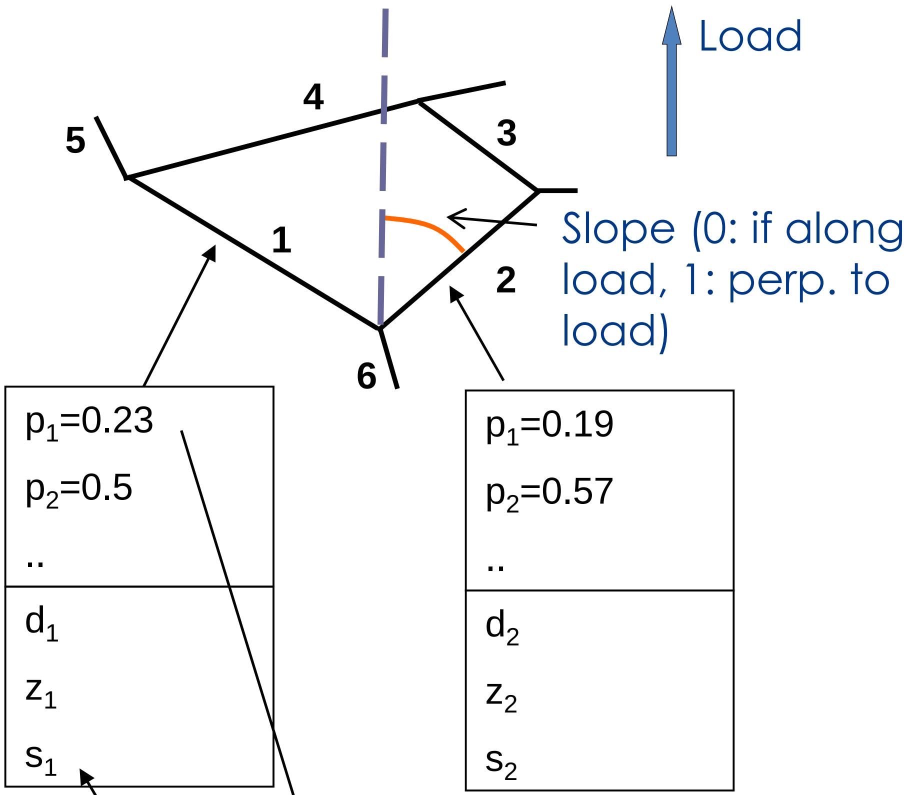
Crack nucleation & short crack growth



If damage > threshold:
→ increase depth z
→ set damage = 0

- Small time steps
- After each step:
  - Accumulate damage of each edge (time, influence of neighbours)
  - If damage > threshold: increase z, set d=0.
- Interaction of neighbours increases crack growth
- Crack consists of entire edges
- If crack growth fast enough: switch to long crack growth model

Crack nucleation & short crack growth

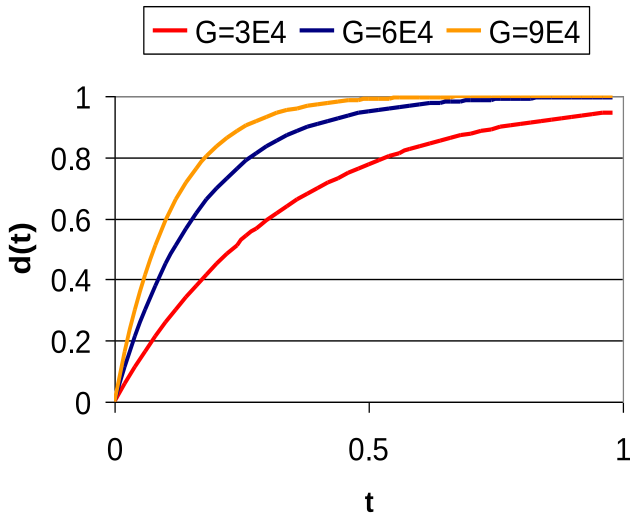


Sensitivity of edge i:

$$s_i = p_1^{a_1} \times p_2^{a_2} \times \mathrm{K} \times p_N^{a_N}$$

- User can define properties for each edge, in examples:
  - Misorientation (p1)
  - Boundary slope (p2)
  - Si concentration (p3)
- Properties set automatically using various random distributions or calculated or read in.
- In addition each edge (i) has a:
  - Depth: z
  - Damage: d
  - Sensitivity: s
- Sensitivity calculated using exponents a1,... aN provided by user

Short crack model



- Time evolution of damage:

$$d_i(t) = 1 - e^{-G \cdot s_i \cdot t}$$

G: Growth

- Influence of neighbours:

C: Coupling

$$d_i = d_i + C \times s_i \Delta t \Delta \bar{z}$$

Average of depth differences (all neighbours)

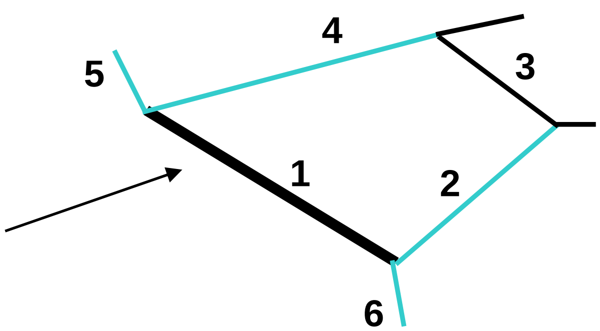
- Edge cracks if:

T: Scaling of Threshold

$$d_i \geq \frac{T}{M}$$

Then: increase z_i and set $d_i = 0$

Material factor (depends on load)

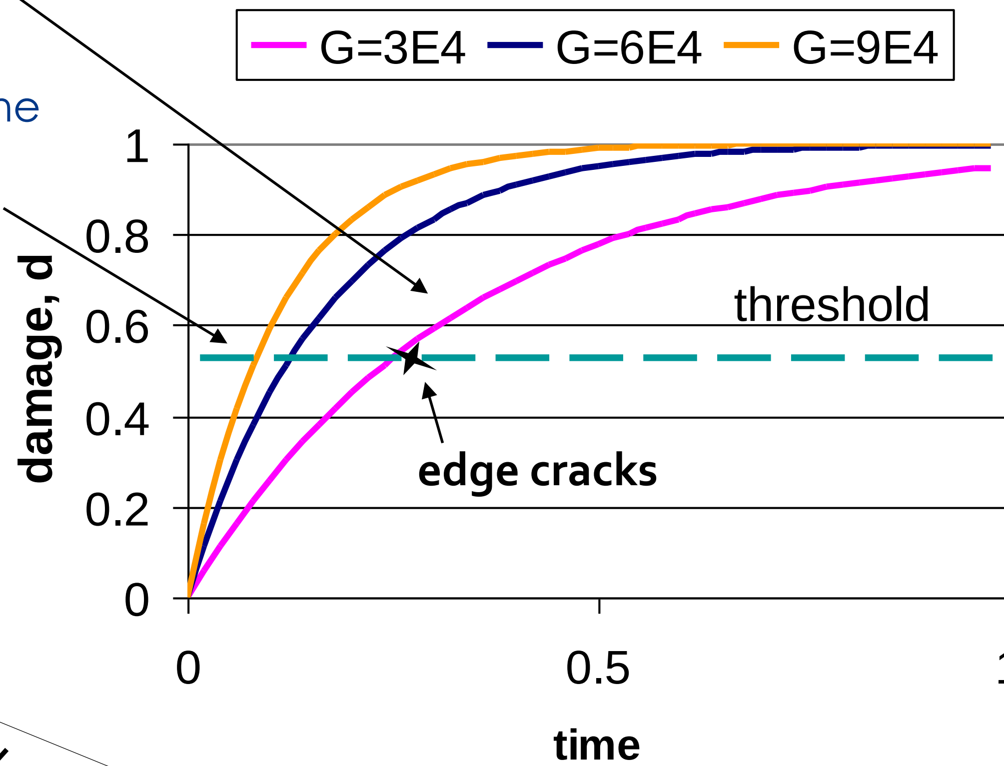


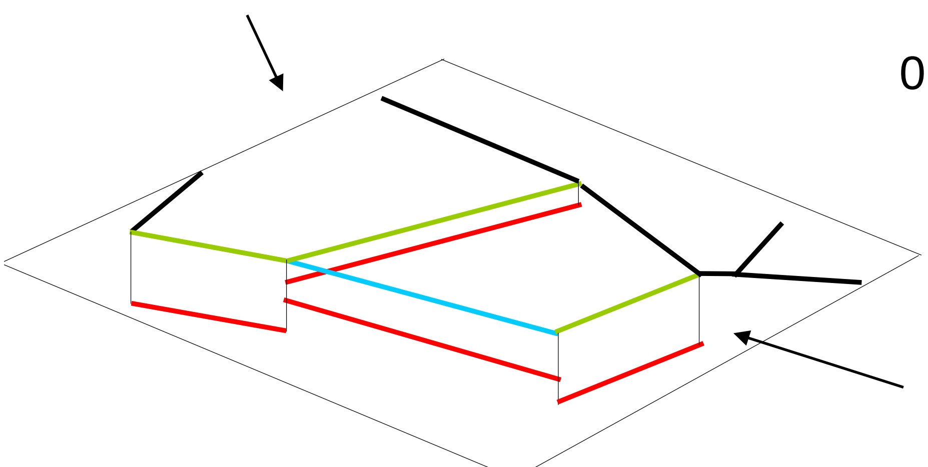
Short crack model parameters

__DamageGrowthRate (G):__ the bigger G the faster damage grows.

__ScaleDamThreshold (T):__ the bigger T the longer it takes for the edge to crack.

__InfluenceNeighbours (C):__ the bigger C the faster damage will grow when any neighbouring edges are cracked deeper.



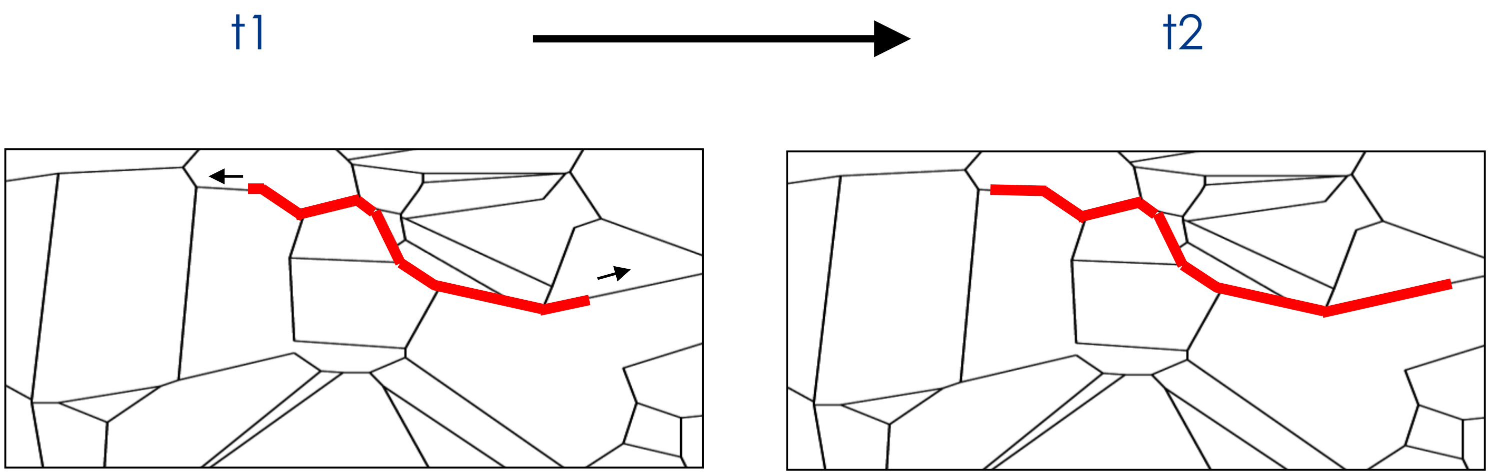


Green = neighbours of blue

Long crack model

If crack grows fast enough then automatic switch to long crack model:

- Damage no more used
- Crack ends move along edges according to fracture mechanics



Long crack model, cont'd

- Long Crack Growth Rate formula

$$CGR = 10^{B_0 + B_1 \cdot Si + B_2 \cdot Cr + B_3 \cdot Y} \cdot K^{2.5}$$

BulkSi
or from mesh

BulkCr
or from mesh

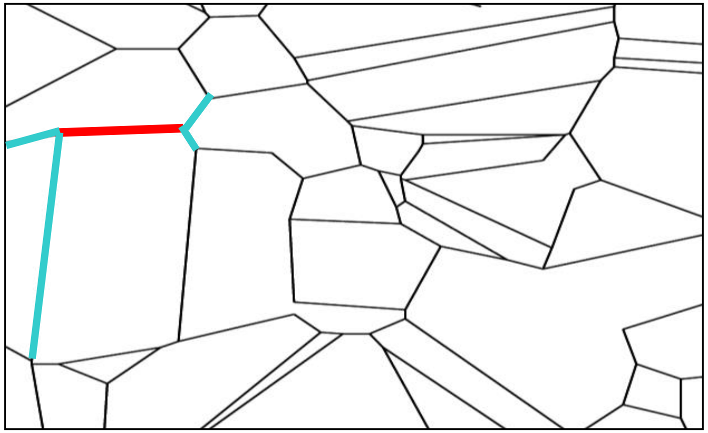
Yield

- Default values of parameters B_0… B_3 have been derived by fitting experimental data. K = stress intensity factor
- Note: If Cr/Si properties defined in mesh, then they will overwrite the *BulkSi*/*BulkCr* parameters

How to determine new properties for GB's below the surface ?

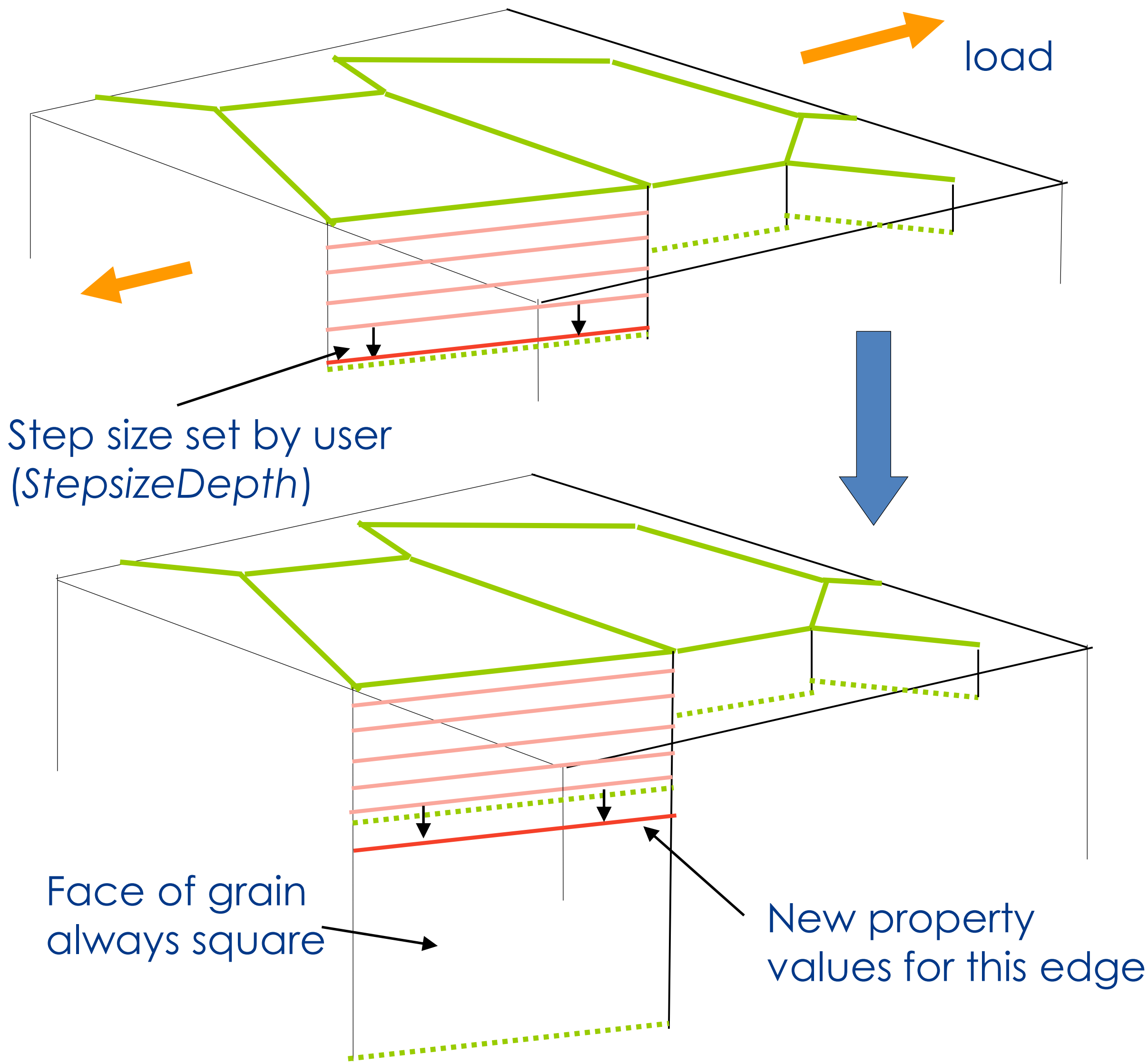
User needs to choose one of 3 schemes (in mesh file):

- ❑ Resample (default): value of edge chosen randomly from entire surface or from neighbours



- ❑ Random: Resample using specified distribution.
- ❑ Binned:
  - At start: calculate probability that edge with property value X has neighbour with value Y
  - Sample from this distribution to get new value for edge.
  - → Statistical variation of property but following distribution on surface.

Growth into depth past grain boundaries



<u>Short Crack growth</u>

- Small steps into depth whenever damage reaches threshold
- Edge properties re-sampled when boundary in 3rd dimension (dotted line) is reached.

<u>Long Crack growth</u>

- Simultaneous growth along surface and into depth based on fracture mechanics.

Shielding and interaction

- Crack nucleation is suppressed close to the sides of existing cracks. To this end influence zones around cracks are used (and controlled in the input file)

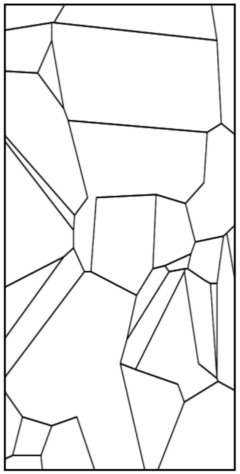
- Cracks that grow close to each other are accelerated and are likely to be merged. ‘Closeness’ defined through influence zones (controlled by input parameters)

Modelling irradiated materials

No parameter specifying level of irradiation. Instead: set %Si, %Cr and yield stress depending on irradiation (dpa)

- Specify distributions of Si/Cr properties either
  - using parameters *BulkSi/BulkCr* or
  - in mesh file. Actual values sampled from distributions:

```
"Si" Normal(4.5, 0.45)
"Cr" Normal(10.5, 1.1)
```



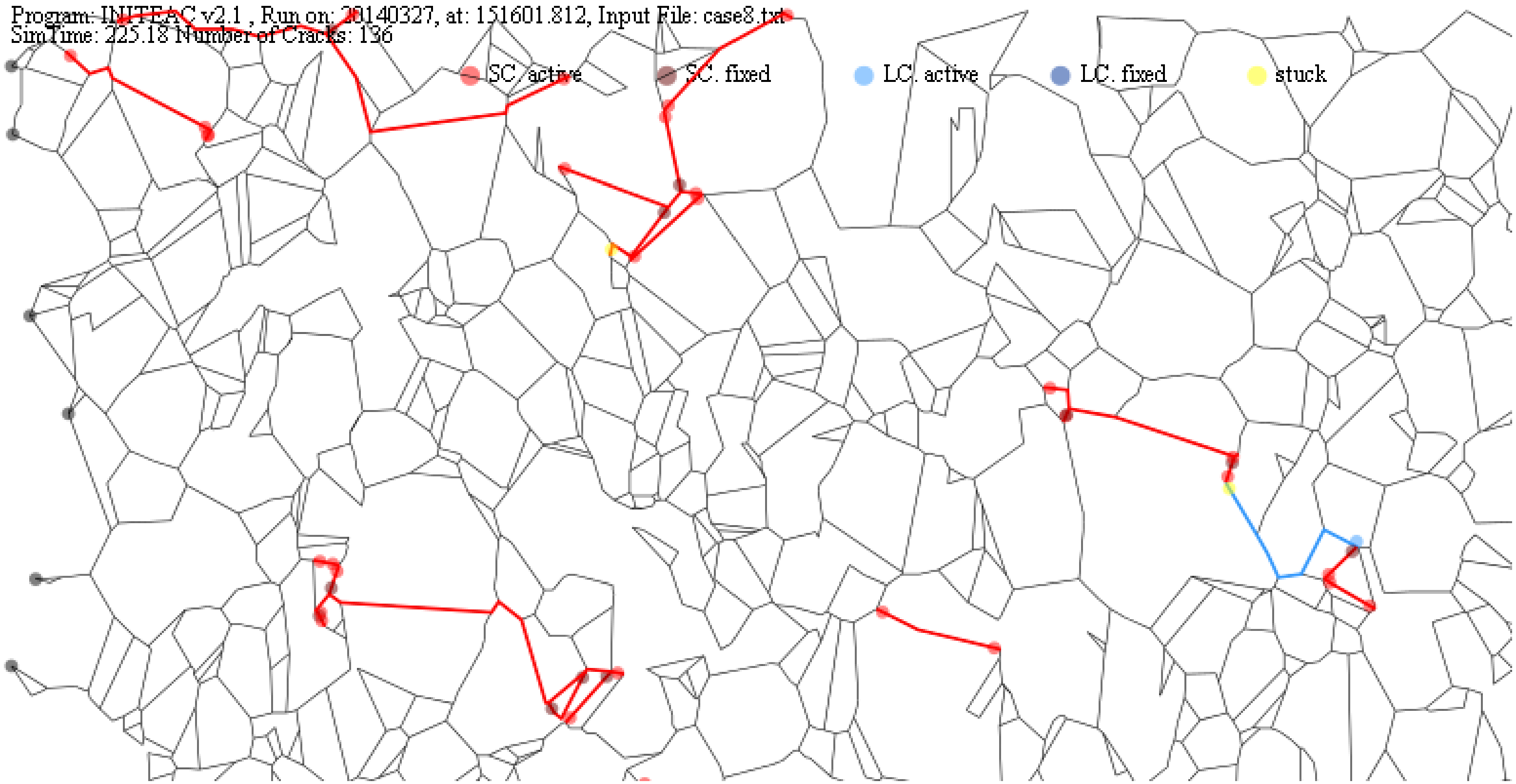
- Specify yield stress (hardening) in input file (*Yield*)

Analysis of INITEAC results

- Run it
- Visualize cracks on grain mesh using graphics **svg** results file.
- Histograms of crack lengths

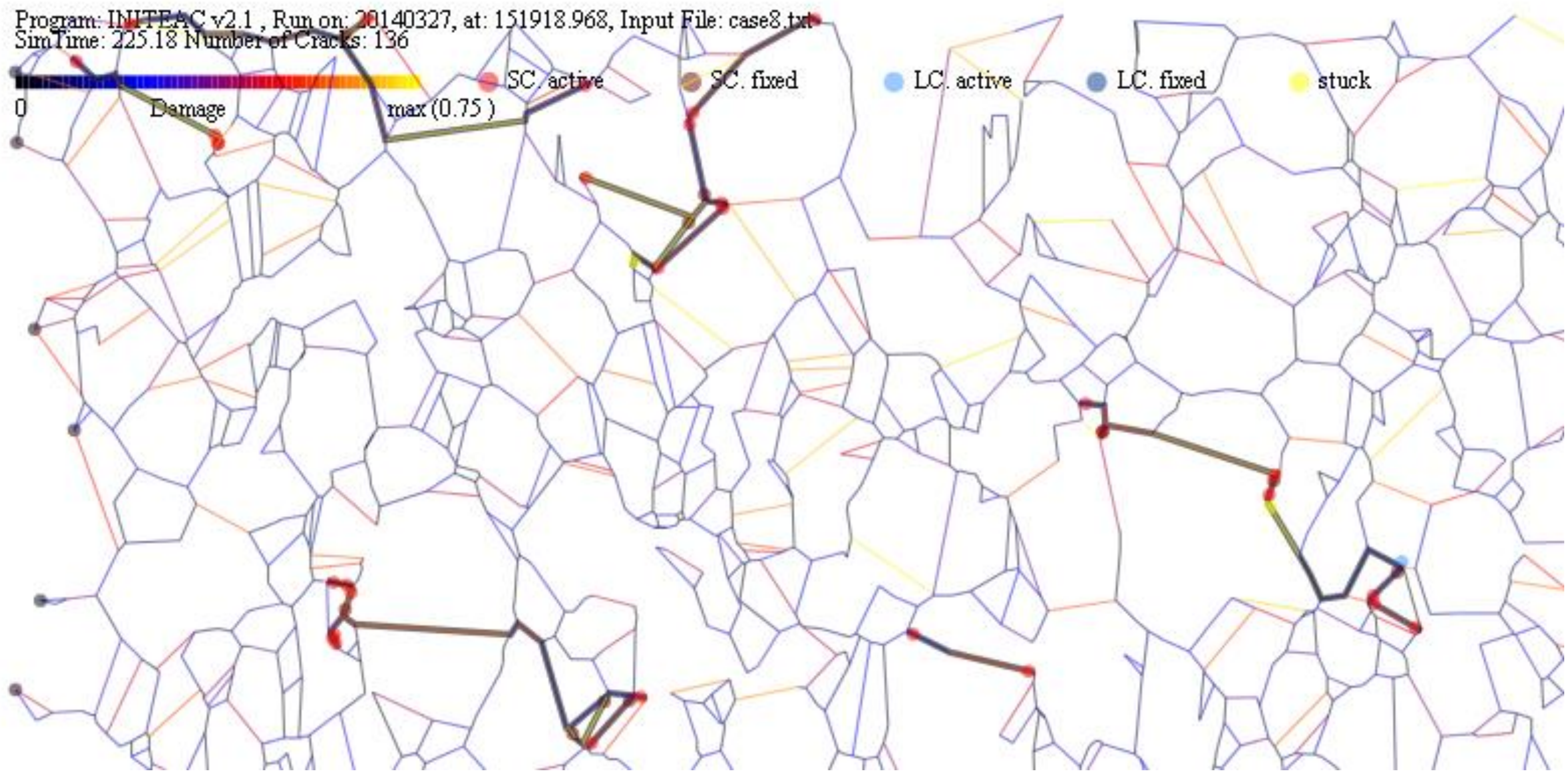
INITEAC output (svg) file

DisplayDetail = 0 (cracks)



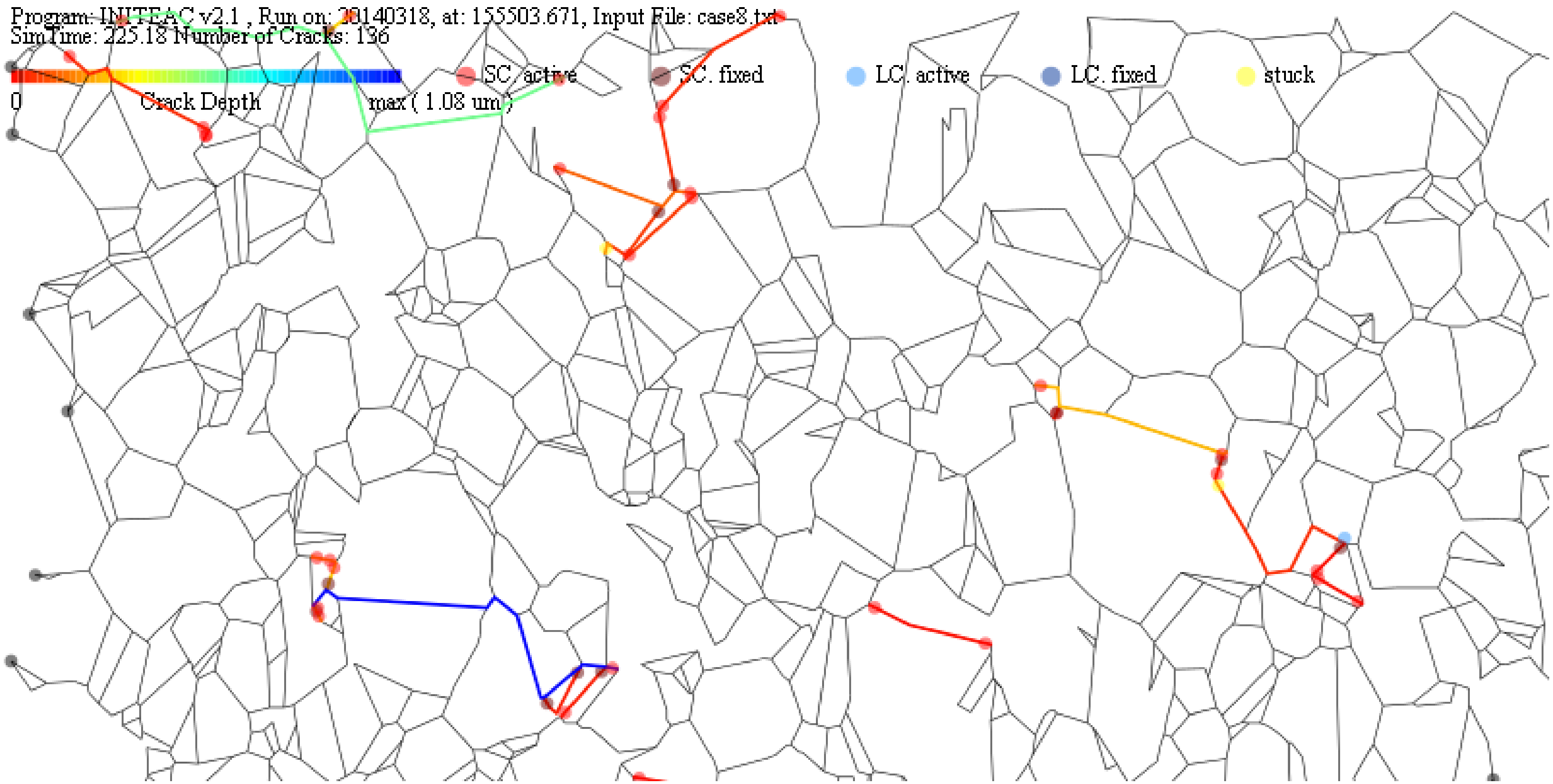
INITEAC output (svg) file

DisplayDetail = 1 (damage)



INITEAC output (svg) file

DisplayDetail = 4 (crack depth)



Summary

- INITEAC = statistical modelling of IASCC
- Based on 2D surface grain mesh
- Internal oxidation / slip development modelled via damage accumulation model
- Stress intensity factor based model for long cracks
- Algorithms for shielding, interaction and coalescence
- 2.5D approach: approximate representation of full 3D grain structure
- Irradiated material modelled by providing corresponding values for Si, Cr, yield stress

- Various output options (depth, damage, crack properties)
- Automatic generation of histograms

.. and now it's your turn !

- INITEAC is set up on your computers together with cases to start from.
- Aim: vary a few parameters and run INITEAC to see how results can be controlled.
- Parameters to play with:
  - Number of INITEAC runs (differing only by random number seed)
  - Damage growth (G)
  - Influence of neighbours (C)
  - Scaling of threshold (T)
  - Load
  - Sensitivity formula
  - Yield stress
  - Si, Cr levels

Example cases

- Open presentation on you computer
- You will find further notes on how to run INITEAC
- 12 example cases to work through. For each case a ‘button’ starts analysis.
- Results are analysed using graphics output (svg file) and histograms

- Have fun ..