Multiscale modelling strategy for predicting fatigue life of steels

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Outline

1. Research background
2. Experimental observation
3. Model development
4. Validation of the model
5. Summary

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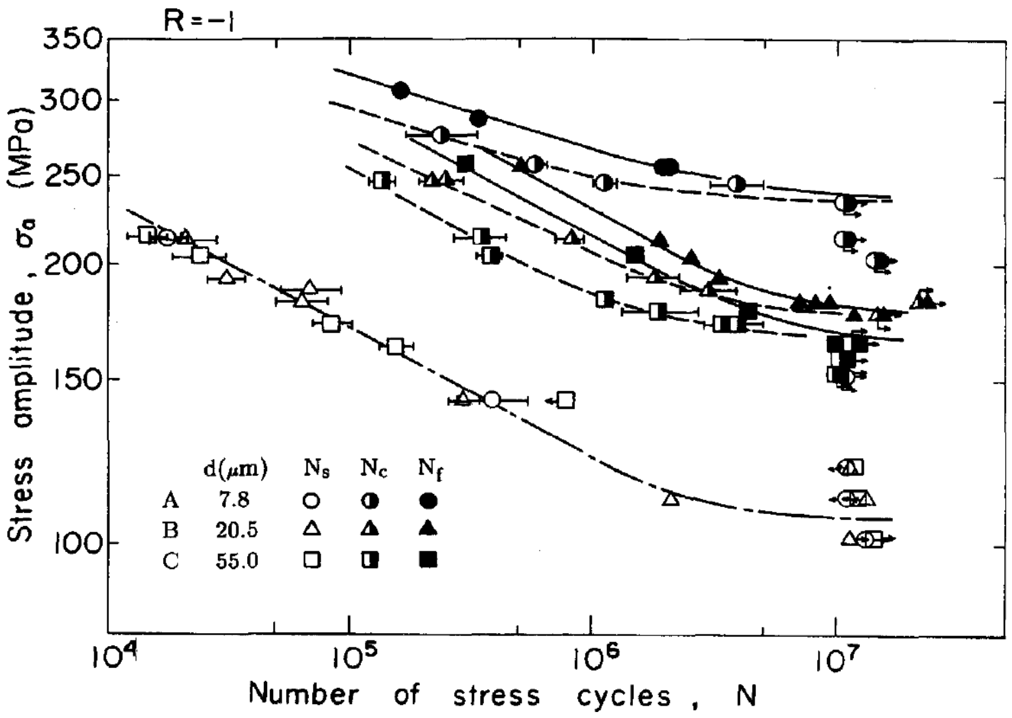
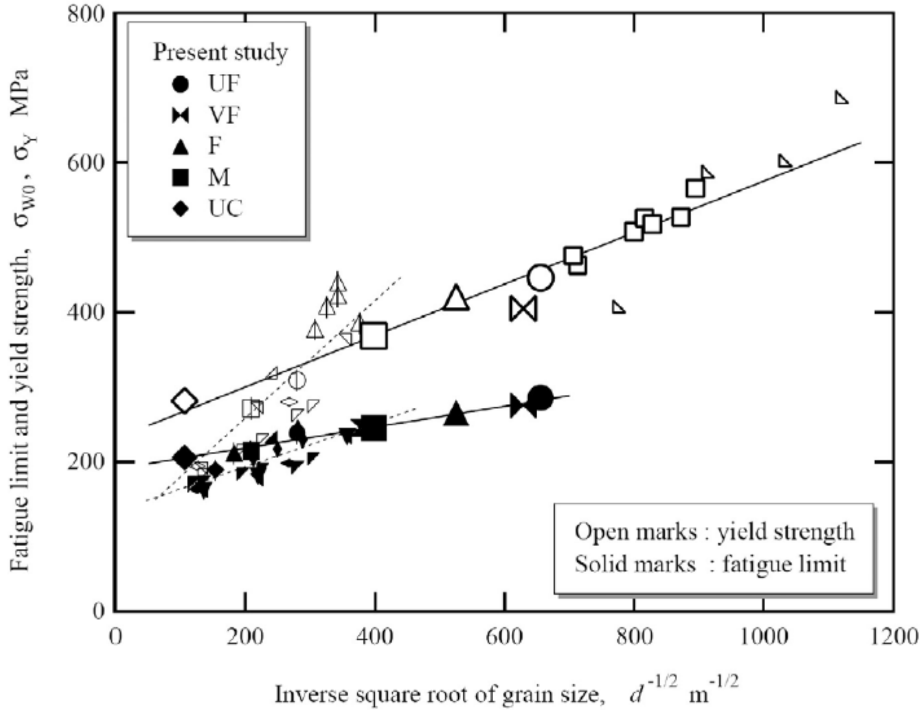
Influence of microstructure on fatigue life



Dependence of fatigue life on grain size*



Influence of grain size on fatigue limit**

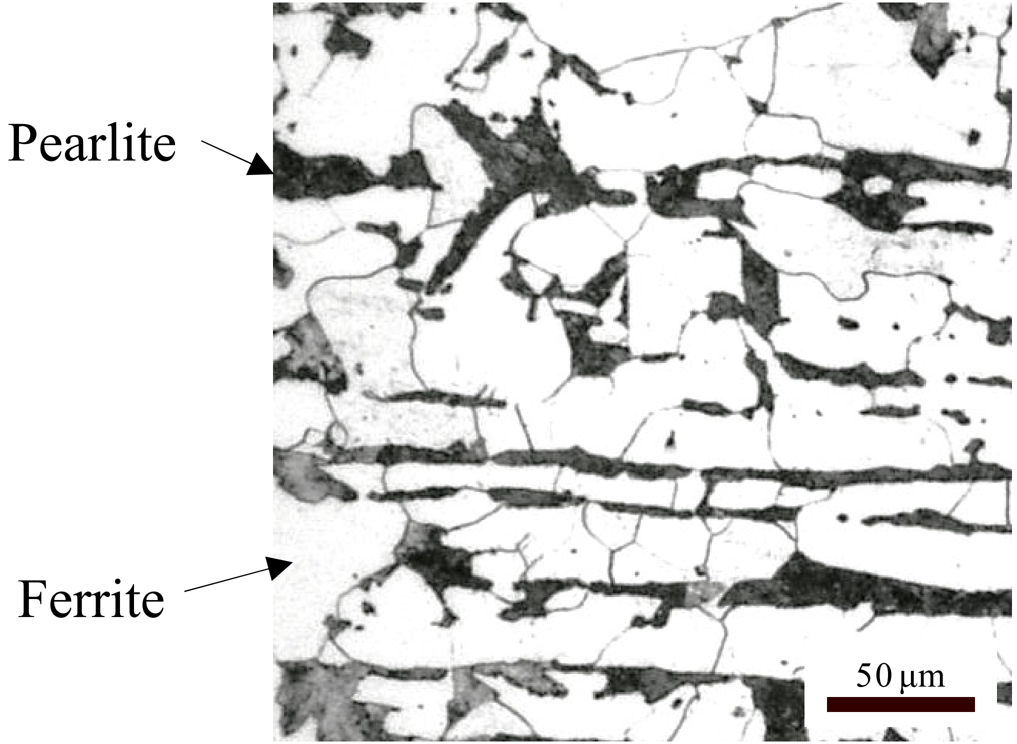
No theory/model to quantitatively explain the influence of microstructure on fatigue life

*Taira et al., Grain-size effect on crack nucleation and growth in long-life fatigue of low-carbon steel, ASTM STP 675 (1979) 135-173.
**Tanaka, Improvement of metal fatigue strength by grain refinement and residual stresses, Reports Faculty Sci. Tech. Meijo Uni. 48 (2008) 67-70.

Objective of the present study

Ferrite-Pearlite Steel

- Most widely used as structural steel
- Two-phase banded microstructure



Development of a model for predicting fatigue life and limit based on microstructural information

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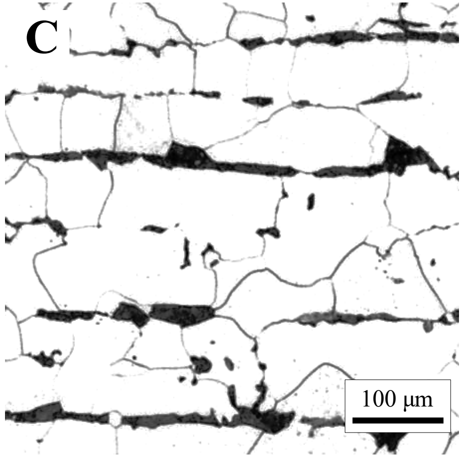
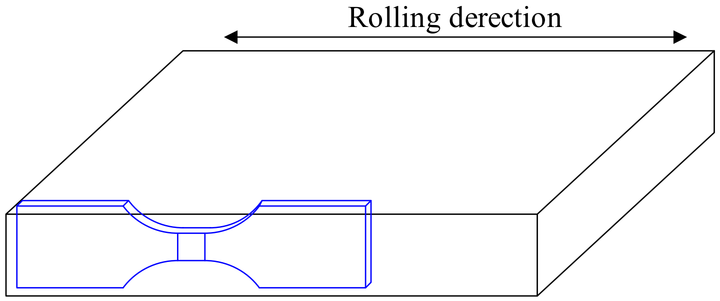
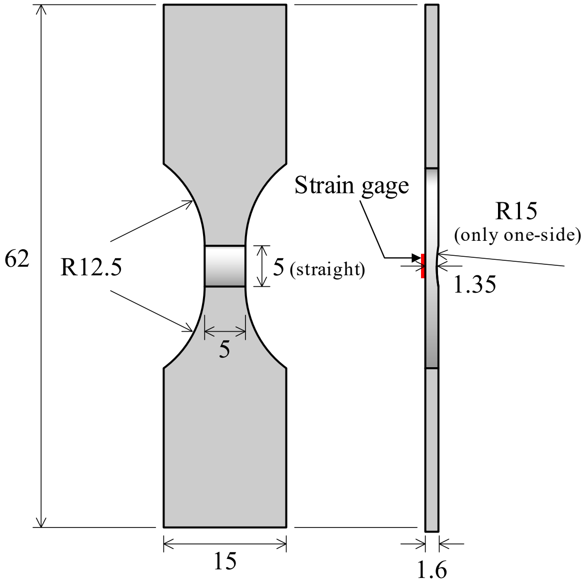
Test and observation conditions





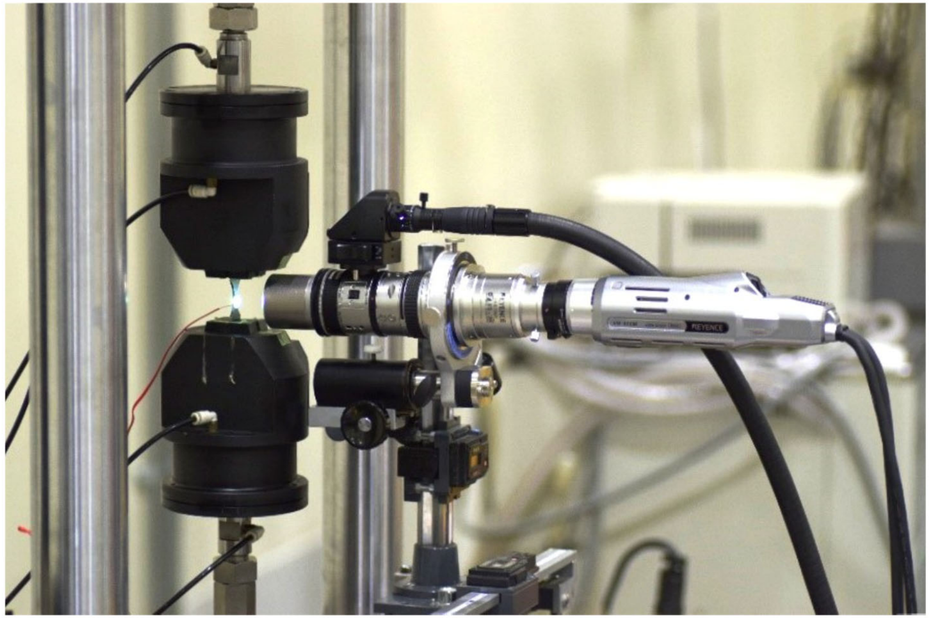
Sampling direction



Tension/compression test using smoothed specimen

Loading condition

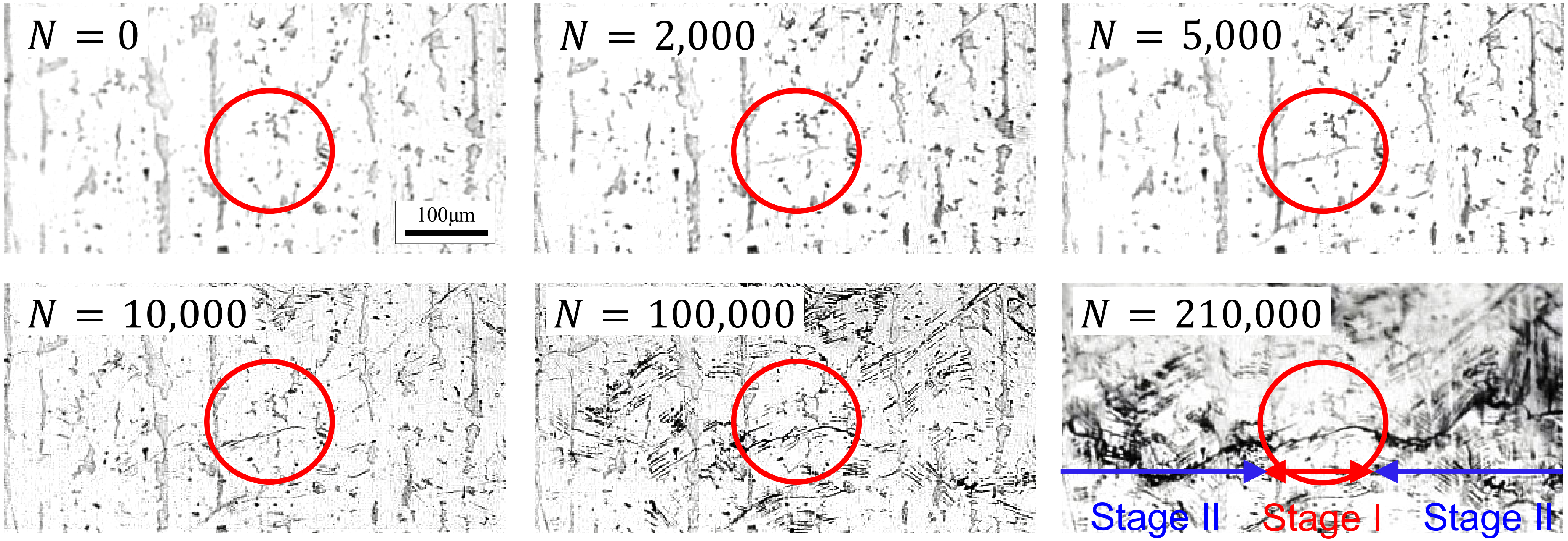
Stress amp. : 150MPa
Stress ratio : −1
Frequency : 10Hz



Observation on crack initiation and growth process

Observation results

Crack initiation site ($N_f = 218{,}987$)



- A “crack” is clearly observed for less than 1% of fatigue life.

  ⇨ It is difficult to define crack initiation life in high cycle fatigue of steels.

- Damage caused by activation of multiple slip systems clearly increased after the crack tip passed the first grain boundary.

  ⇨ Stage I and Stage II may be defined by the first grain boundary.

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Modelling concepts

Relationship between microstructure and fatigue life and limit

- Input: Microstructural information ⇨ Output: Fatigue life and limit

Calculation on fatigue life

- It was difficult to define “crack initiation” life.
- Entire fatigue life is estimated **from “crack growth” life alone**.

Reducing dimension of the problem

Fatigue crack initiation and growth: **Complicated 3D phenomenon**

Characteristic features:

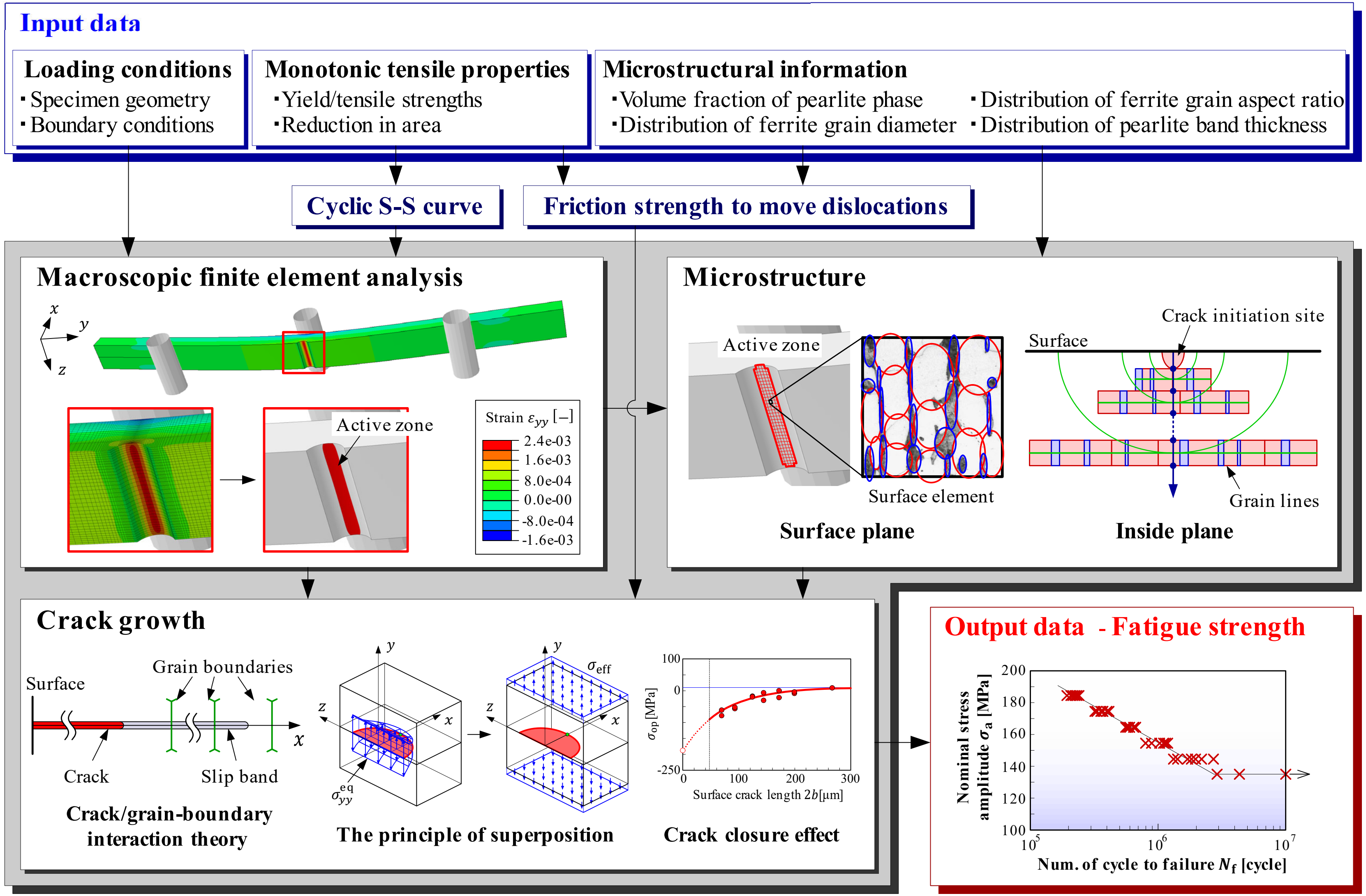
- A crack generally initiates at a surface.
- Crack growth direction is approximately orthogonal to that of the maximum principal stress.

⇨ **“2D problems with two steps”**

Multiscale model synthesis

- Integrating multiple models with large scale differences

Outline of the proposed model



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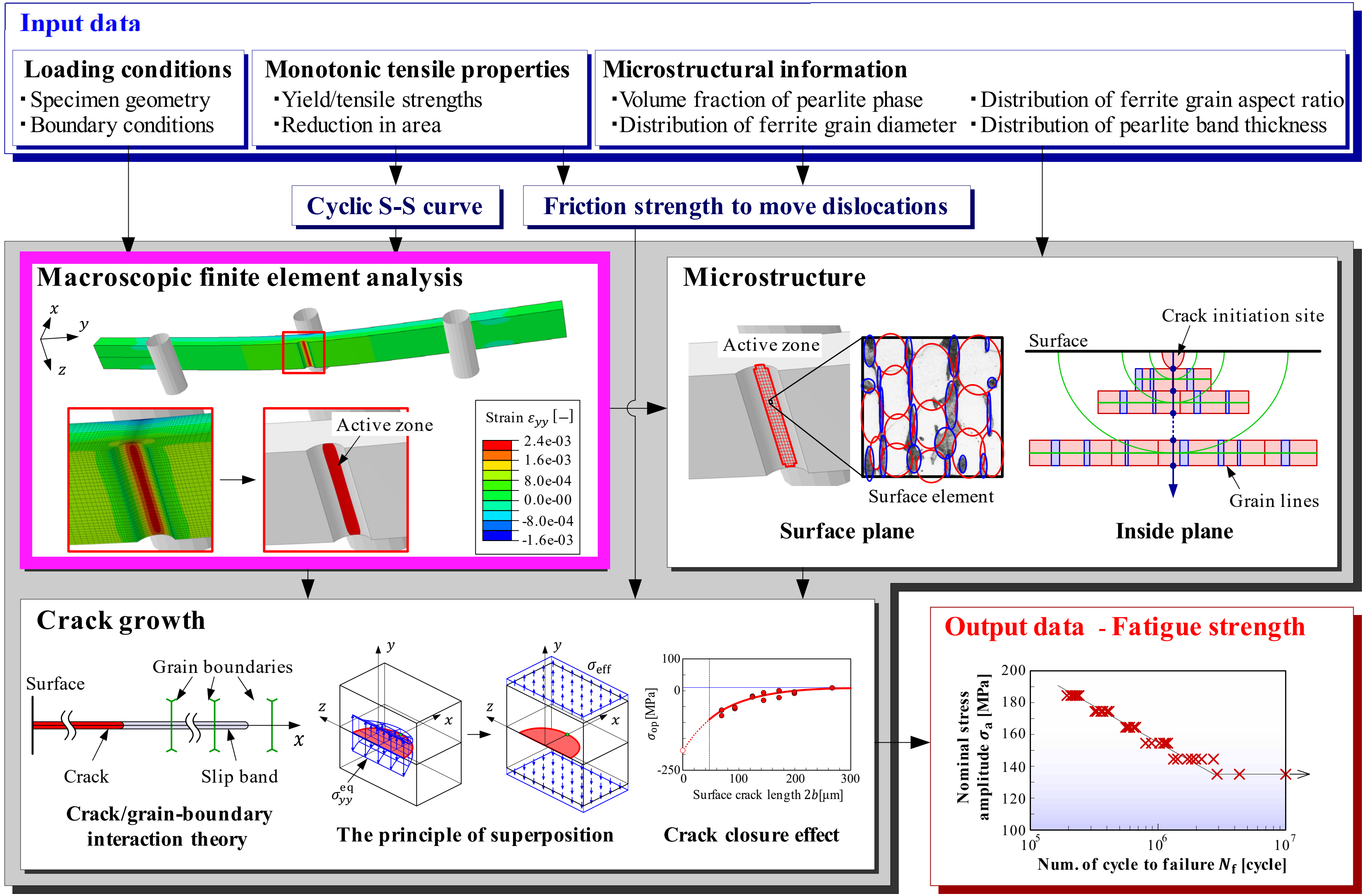


Model of finite element analysis

Role of model of FEA:
Calculation of strain amplitude field and definition of an active zone

Cyclic stress-strain relationship:
Empirical formula by Li et al.*

$$\varepsilon_{\mathrm{eq}}^{\mathrm{a}} = \varepsilon_{\mathrm{e}}^{\mathrm{a}} + \varepsilon_{\mathrm{p}}^{\mathrm{a}} = \frac{\sigma_{\mathrm{eq}}^{\mathrm{a}}}{E} + \left(\frac{\sigma_{\mathrm{eq}}^{\mathrm{a}}}{K}\right)^{\frac{1}{m}}$$

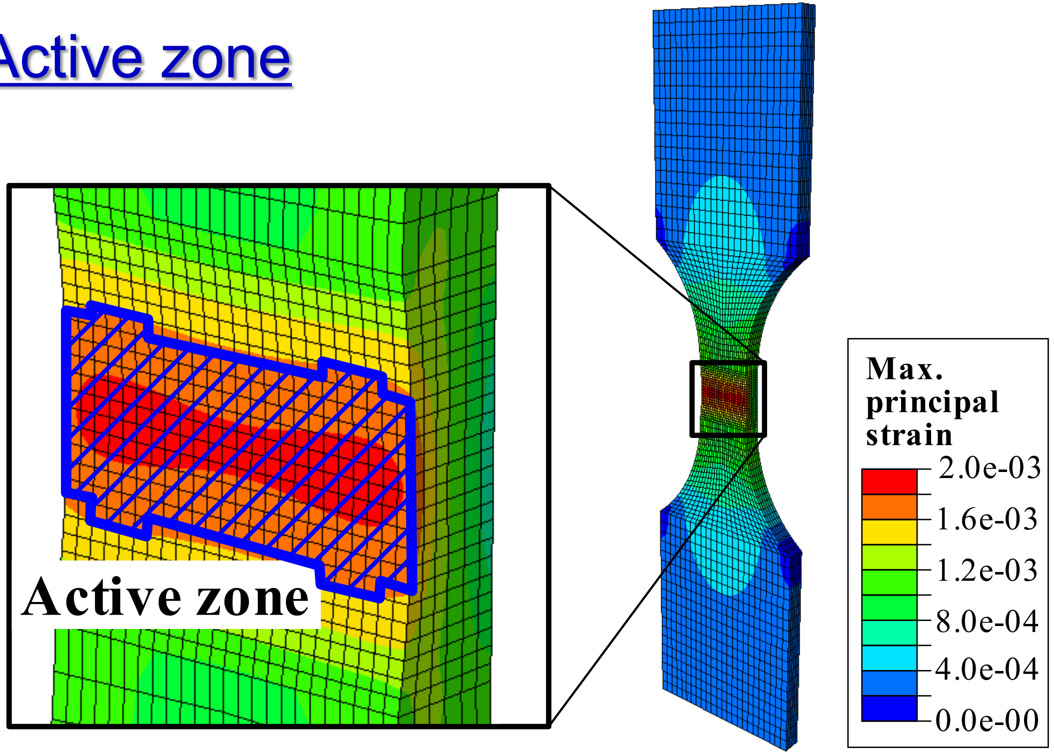
$\varepsilon_{\mathrm{eq}}^{\mathrm{a}}$: equivalent strain amplitude
$\sigma_{\mathrm{eq}}^{\mathrm{a}}$: equivalent stress amplitude

Input data: Only monotonic tensile properties

σ_{B}: tensile strength
σ_{Y}: yield strength
r_{A}: reduction area

*J. Li et al., An improved method for estimation of Ramberg-Osgood curves of steels from monotonic tensile properties, Fatigue Fract. Eng. Mater. Struct. 39 (2016) 412-426.

Active zone



- Defined as a surface domain where a crack is possibly initiated based on strain amplitude filed

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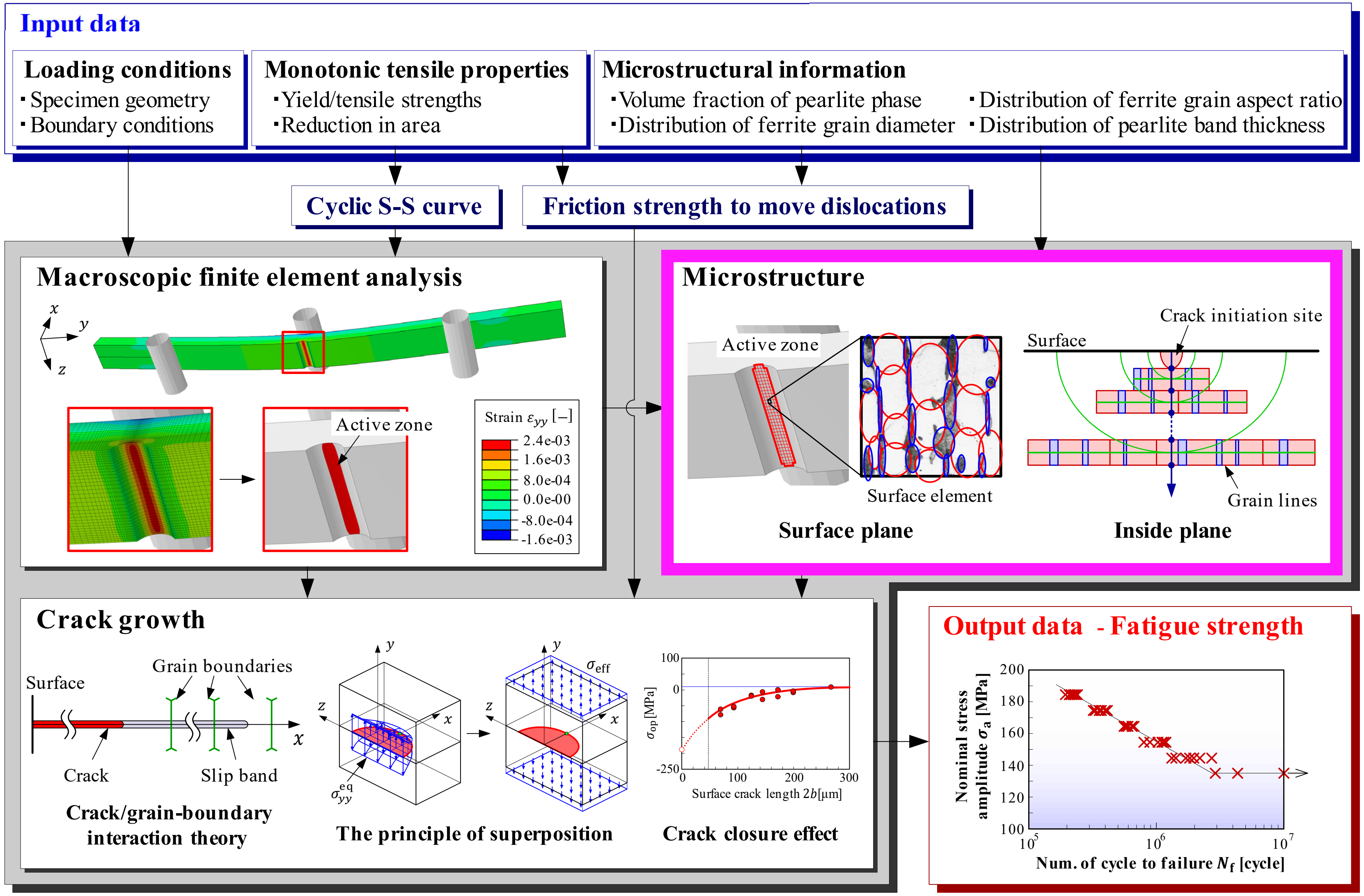
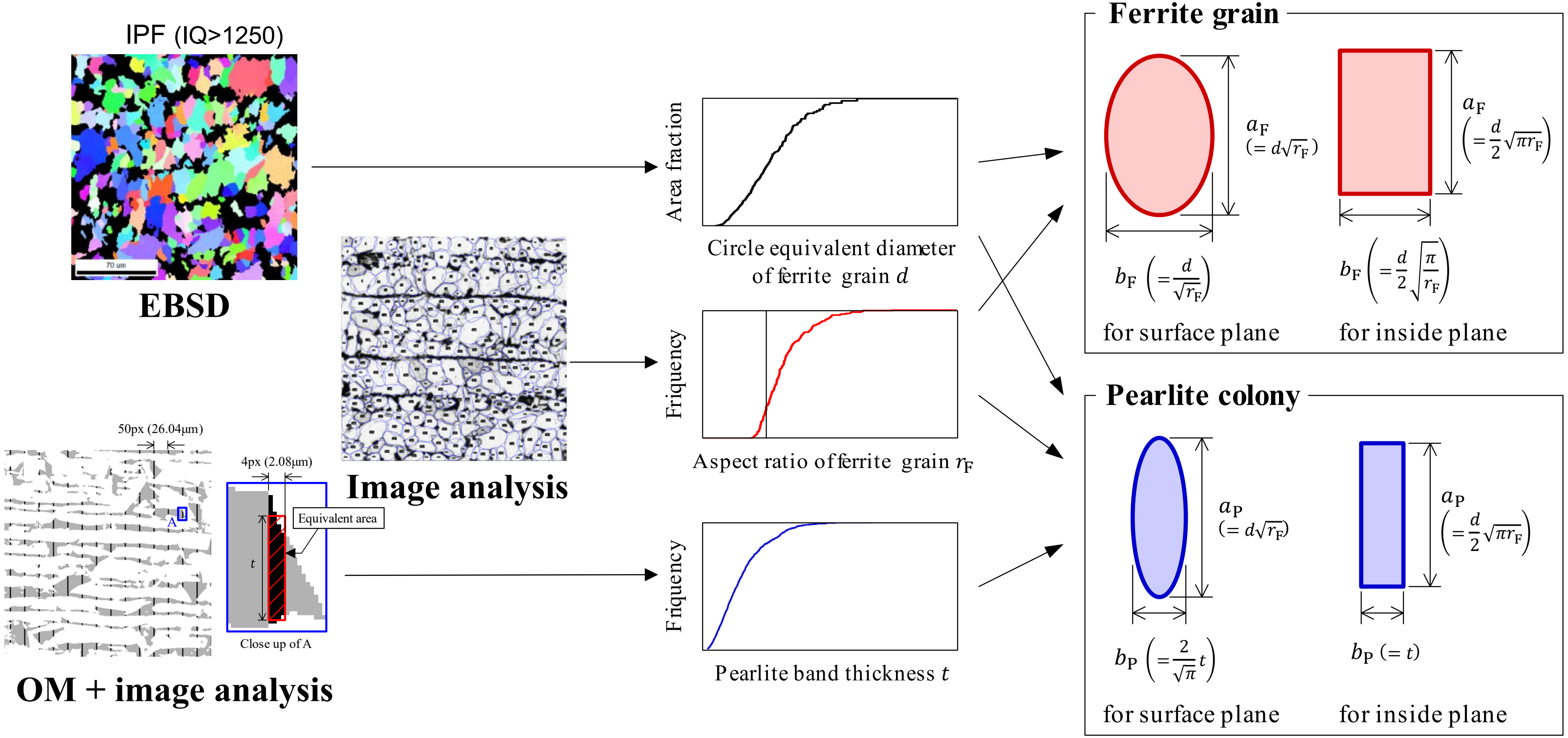


Geometries of ferrite grains/pearlite colonies

2D assumption ➡ Simplification on microstructure modelling



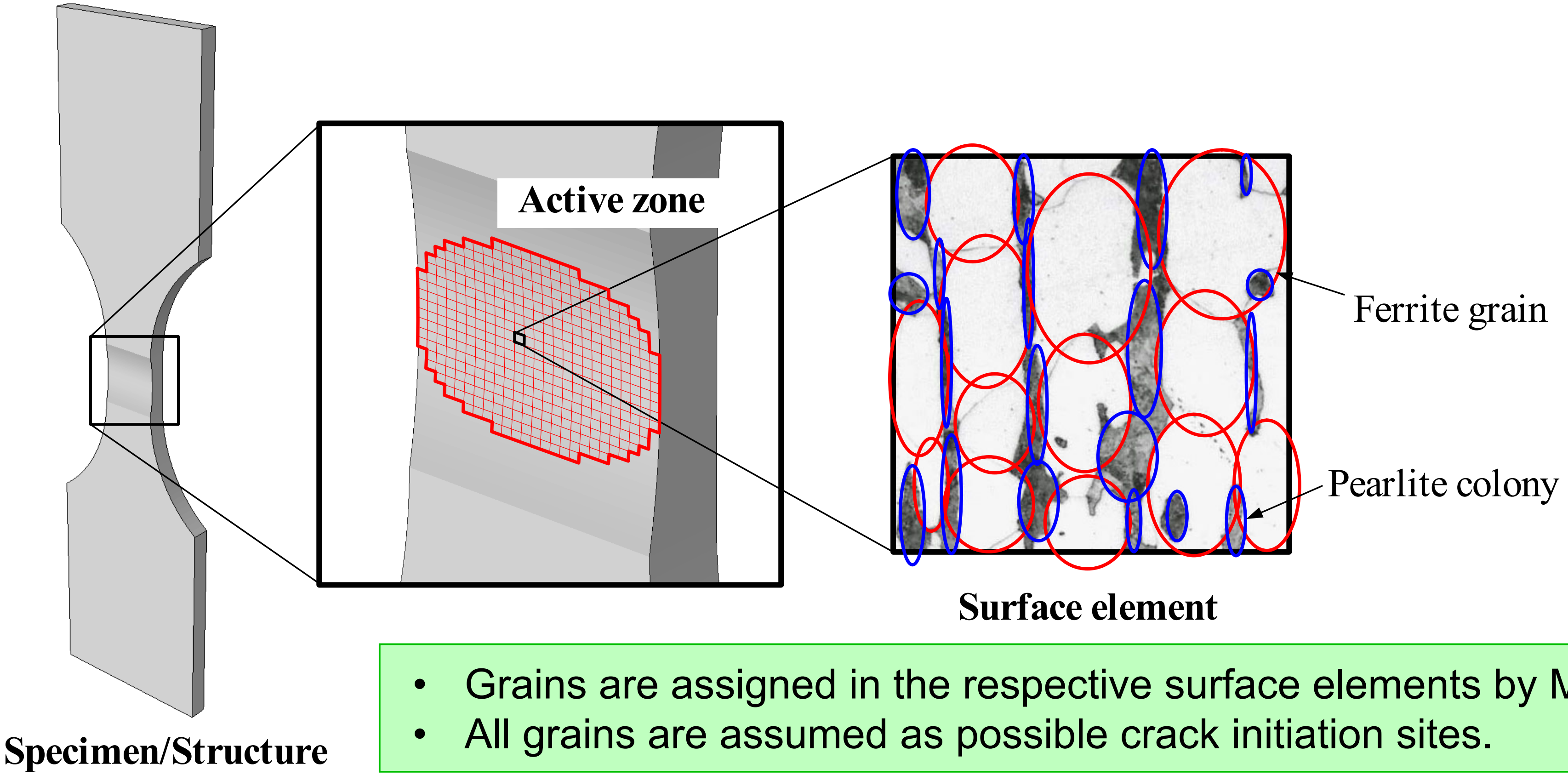
Grain orientation is assigned for each grain

Spatial grain distribution in surface plane

Active zone: Surface plane where a crack is possibly initiated

Surface elements: Simplification of the respective grain locations

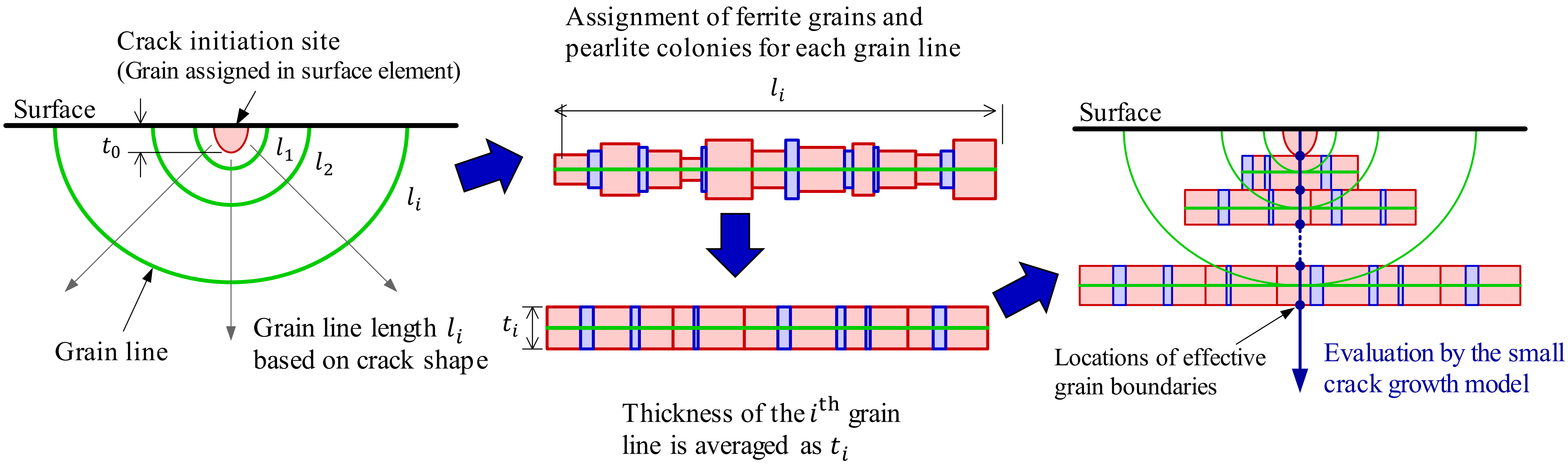
(i.e., the exact location of a grain in an area element is not considered.)



- Grains are assigned in the respective surface elements by Monte Carlo method.
- All grains are assumed as possible crack initiation sites.

Spatial grain distribution in inside plane

Spatial distribution is modelled corresponding to crack shape transition



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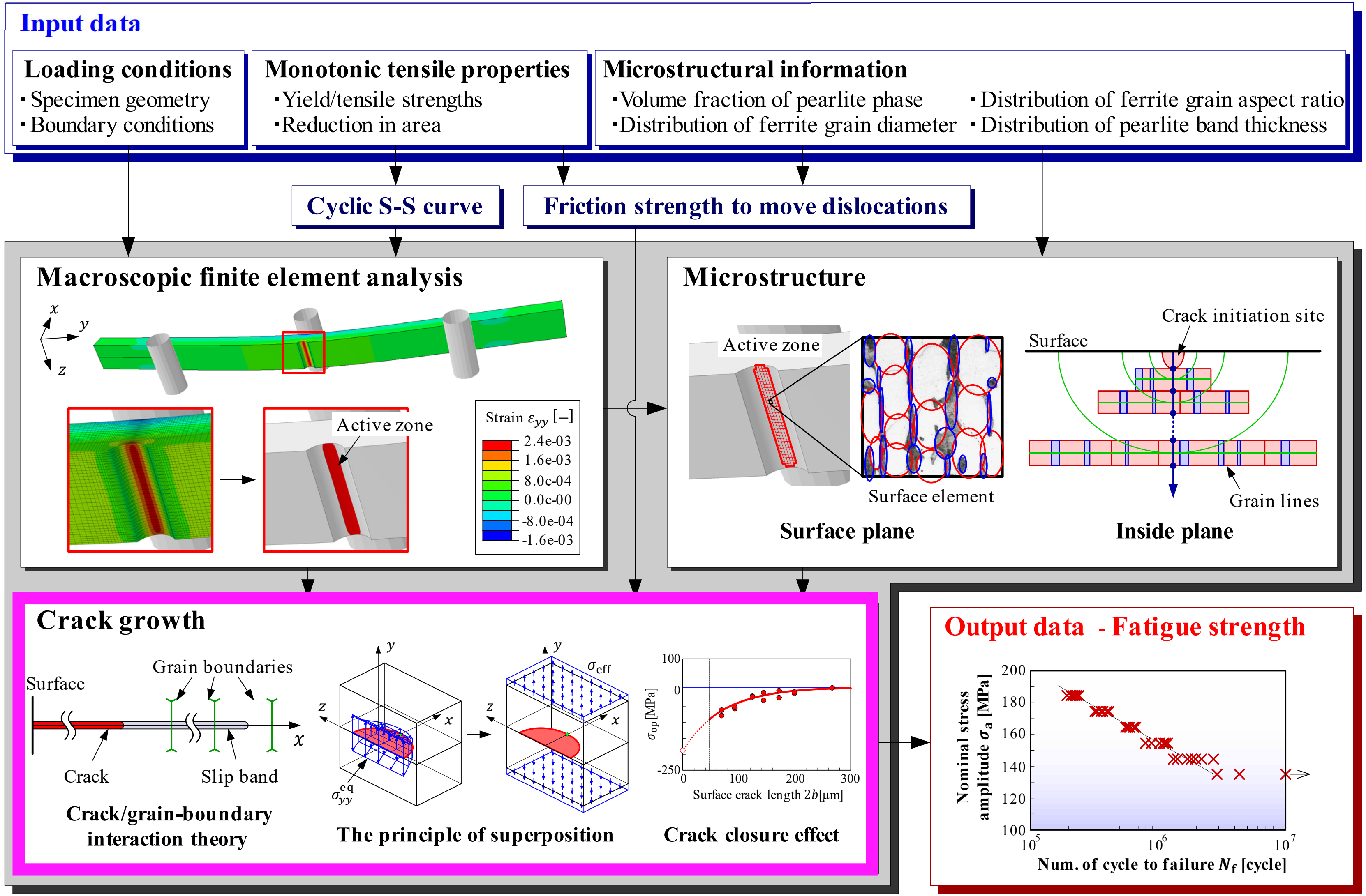


Basic theory

Fatigue life: Calculated from only crack growth simulation

→ **The interaction theory between a crack and grain boundaries***

- Based on Dugdale model and Continuously distributed dislocation theory
- Grain boundary (misorientation) effects

Slip band length c:

$$\frac{\pi}{4}-\frac{\tau_j^{\mathrm{f}}}{\Delta\tau_j}\arccos\left(\frac{a}{c}\right)-\sum_{i=j+1}^{\infty}\left(\frac{\tau_i^{\mathrm{f}}}{\Delta\tau_i}-\frac{\tau_{i-1}^{\mathrm{f}}}{\Delta\tau_{i-1}}\right)\arccos\left(\frac{l_{i-1}}{c}\right)=0$$

Crack tip sliding displacement $\Delta\mathrm{CTSD}$:

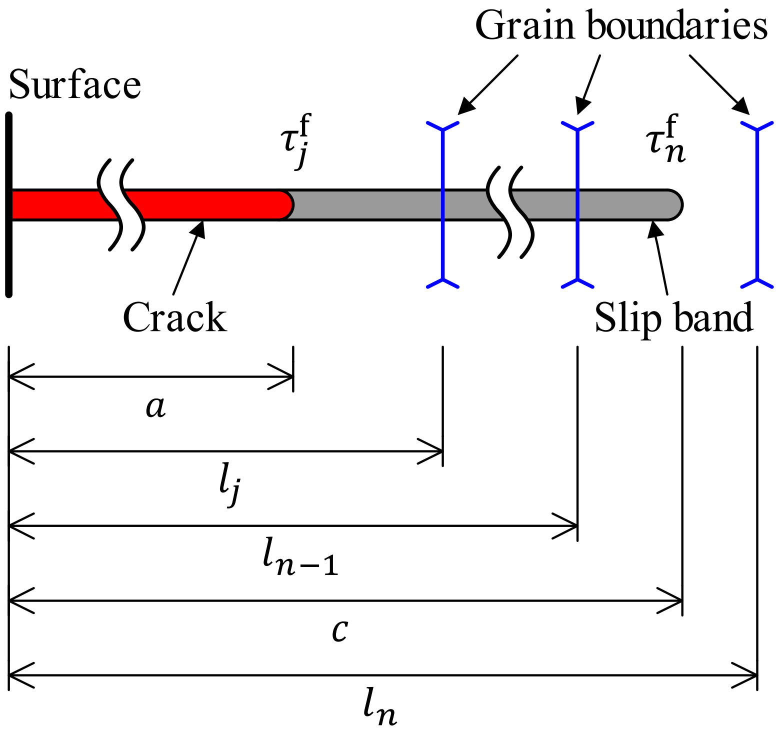
$$\Delta\mathrm{CTSD}=f(a/b)\cdot\frac{4(1-\nu)}{\pi G}\left[2a\tau^{\mathrm{f}}{}_j\ln\left(\frac{c}{a}\right)+\Delta\tau_j\sum_{i=j+1}^{\infty}\left(\frac{\tau^{\mathrm{f}}{}_i}{\Delta\tau_i}-\frac{\tau^{\mathrm{f}}{}_{i-1}}{\Delta\tau_{i-1}}\right)g(a,c,l_{i-1})\right]$$

where $g(a,c,l)=l\ln\left|\frac{\sqrt{c^2-l^2}+\sqrt{c^2-a^2}}{\sqrt{c^2-l^2}-\sqrt{c^2-a^2}}\right|-a\ln\left|\frac{a\sqrt{c^2-l^2}+l\sqrt{c^2-a^2}}{a\sqrt{c^2-l^2}-l\sqrt{c^2-a^2}}\right|$

Crack growth rate $\mathrm{d}a/\mathrm{d}N$:

$$\frac{da}{dN}=C(\Delta\mathrm{CTSD}^n-\Delta\mathrm{CTSD_{th}}^n)$$

Validity is found in the study by Schaef and Marx**



*Tanaka et al., Modelling of small fatigue crack growth interacting with grain boundary, Eng. Fract. Mech. 24 (1986) 803-819.
**Schaef, Marx, A numerical description of short fatigue cracks interacting with grain boundaries, Acta Mater. 60 (2012) 2425–2436.

Basic theory

Fatigue life: Calculated from only crack growth simulation

➡ The interaction theory between a crack and grain boundaries*

- Based on Dugdale model and Continuously distributed dislocation theory
- Grain boundary (misorientation) effects

Input data

- Applied stress range $\Delta\tau_i$
- Friction strength to move dislocations τ_i^{f}
- Grain sizes d_i
- Crack length a

Output data

- Dislocation density
- Slip band length c
- Crack tip sliding displacement range $\Delta\mathrm{CTSD}$
- Crack growth rate $\mathrm{d}a/\mathrm{d}N$
- Fatigue life N_{f}

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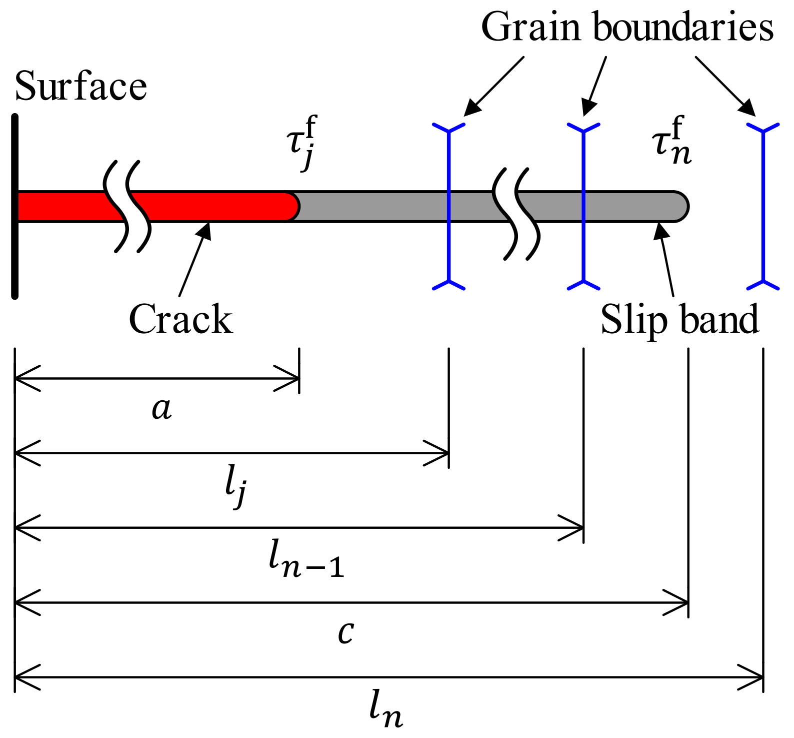

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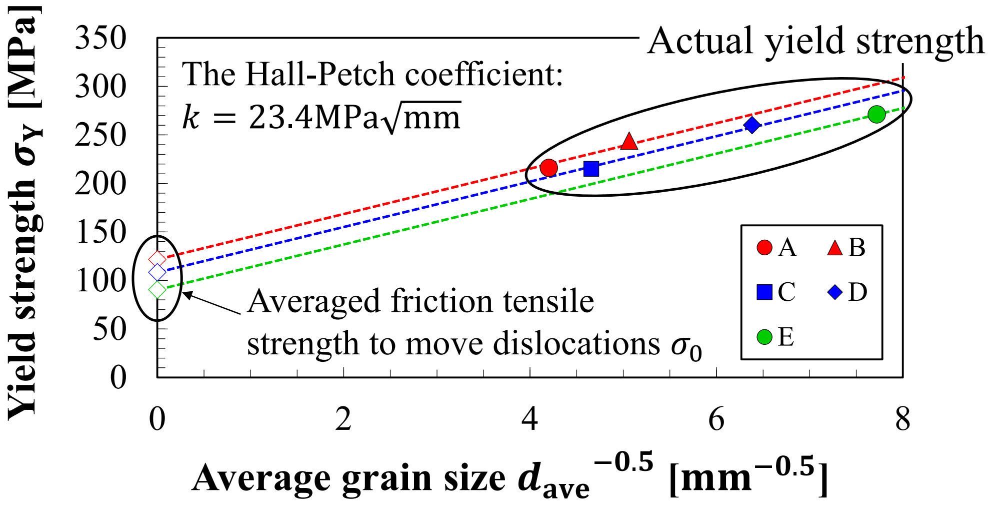
Friction strength to move dislocations (Material resistance)

Material resistance:

Friction strength to move dislocations τ_i^{f} ⇨ Yield shear strength of single crystal

Hall-Petch law

$$\sigma_{\mathrm{Y}} = \sigma_0 + \frac{k}{\sqrt{d_{\mathrm{ave}}}}$$



Friction strengths $\tau_{\mathrm{F}}^{\mathrm{f}}$ (ferrite), $\tau_{\mathrm{P}}^{\mathrm{f}}$ (pearlite)

$$\frac{1}{2}\sigma_0 = \left(1 - V_{\mathrm{f}}^{\mathrm{P}}\right)\tau_{\mathrm{F}}^{\mathrm{f}} + V_{\mathrm{f}}^{\mathrm{P}}\tau_{\mathrm{P}}^{\mathrm{f}}$$ (Linear mixture rule)

$$\frac{\tau_{\mathrm{F}}^{\mathrm{f}}}{\tau_{\mathrm{P}}^{\mathrm{f}}} = \frac{198}{276}$$ (hardness ratio, empirical knowledge*)

*Shoji, Simulation-based method for hierarchal design to improve ductile crack growth resistance of structural component, Int. J. Fract. 192 (2015) 167-178.

Effective shear stress (Driving force)

Driving force: Effective shear stress $\Delta\tau_i$

Equivalent stress tensor corresponding to total strain tensor

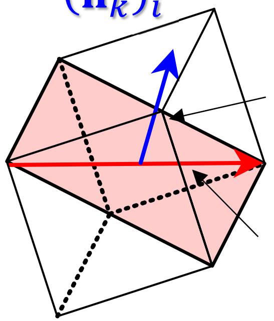
$$\boldsymbol{\sigma}_{\mathrm{eq}} = 2\left(\mathbf{C}_{\mathrm{e}}:\boldsymbol{\varepsilon}_{\mathrm{e}} + \mathbf{C}_{\mathrm{p}}:\boldsymbol{\varepsilon}_{\mathrm{p}}\right)$$

$\Delta\tau_i$ considering slip system of BCC crystal

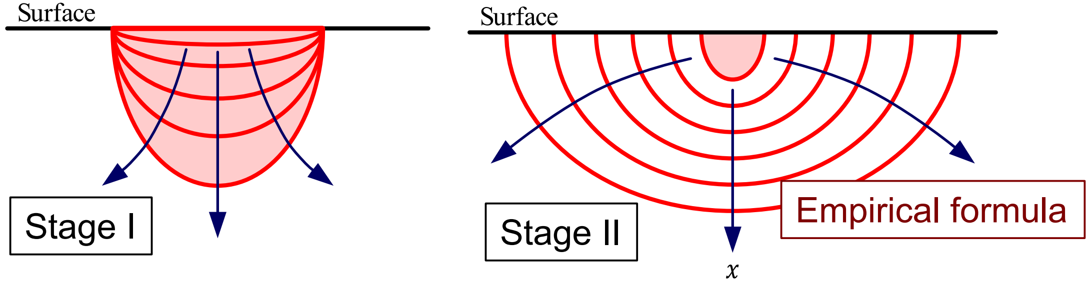
$$\Delta\tau_i = \max_{k=1\ldots6}\left[\max_{l=1,2}\left[(\mathbf{n}_k)_i^{\mathrm{T}}\cdot\Delta\boldsymbol{\sigma}_{i-1}\cdot(\mathbf{m}_{kl})_i\right]\right]$$

where $\Delta\boldsymbol{\sigma}_{i-1} = \begin{cases} \Delta\boldsymbol{\sigma}_{\mathrm{eff}} & (i=j) \\ \Delta\tau_{i-1}(\mathbf{n}_k)_{i-1}^{\mathrm{T}}\times(\mathbf{m}_{kl})_{i-1} & (i \geq j+1) \end{cases}$

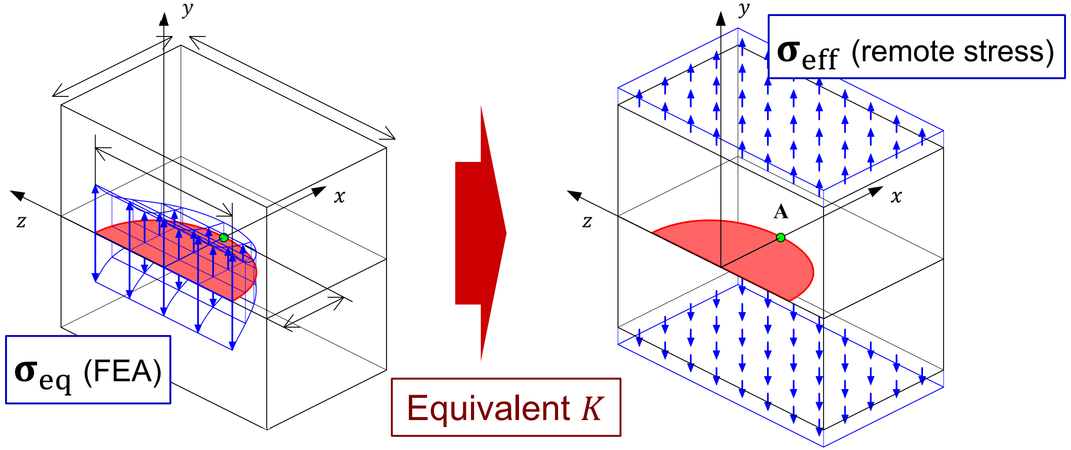
j: grain no. where the crack tip is located



Crack shape



Strain distribution



Crack opening/closure

Effective remote stress tensor range:

$$\Delta\boldsymbol{\sigma}_{\mathrm{eff}} = \boldsymbol{\sigma}_{\mathrm{eff}}[\sigma_{\mathrm{max}}] - \boldsymbol{\sigma}_{\mathrm{eff}}[\sigma_{\mathrm{op}}]$$

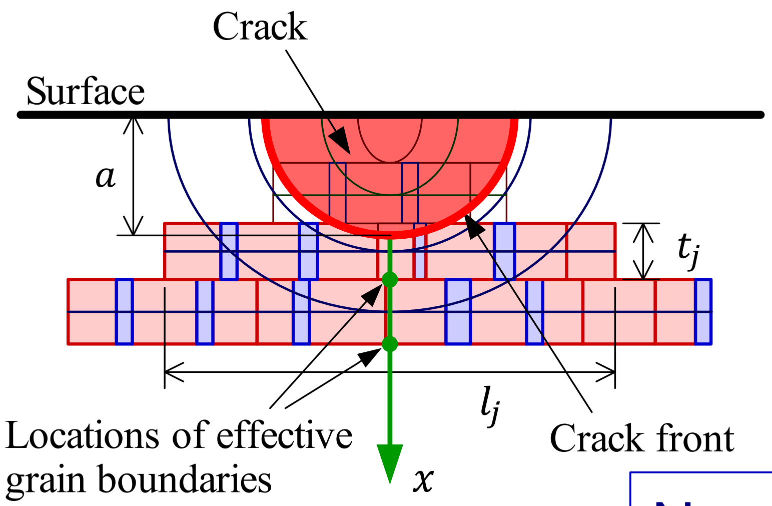
Crack opening stress

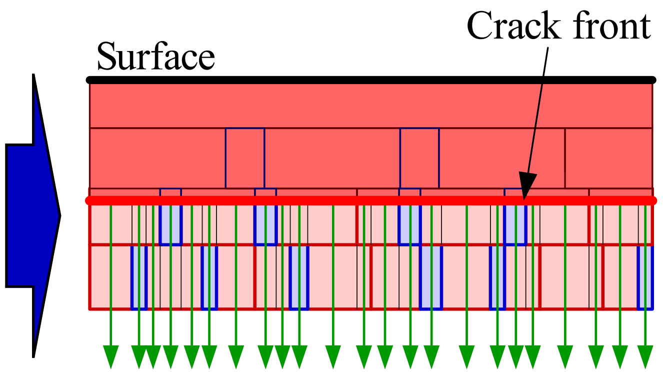
Evaluation of fatigue life

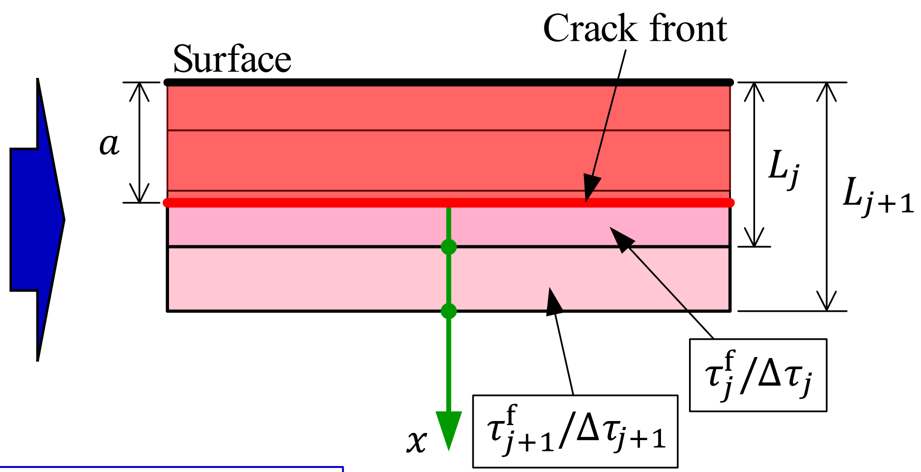
Crack initiation at every grain assigned on surface elements

$\Delta\tau_i$ for all combinations of adjacent grains

Interaction theory between crack and grain boundaries







Normalizing grain lines

Averaging $\tau_i^{\mathrm{f}}\ /\Delta\tau_i$

Fatigue life of the specimen N_{f}:
the minimum number of cycles to failure at all the crack initiation sites

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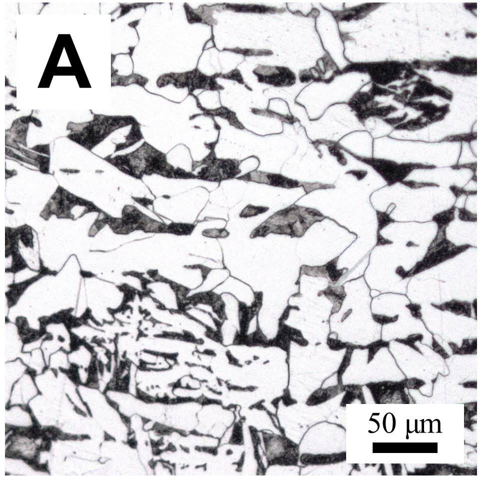
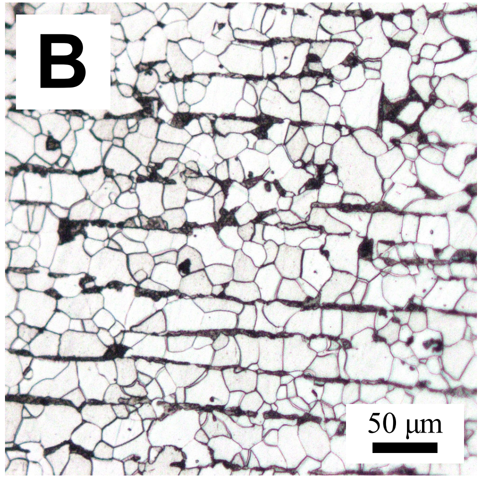
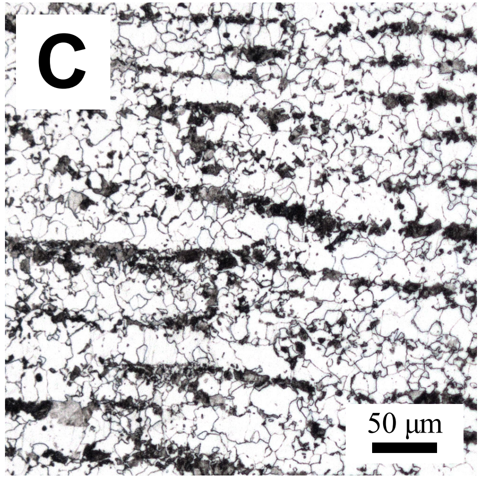
Test steels







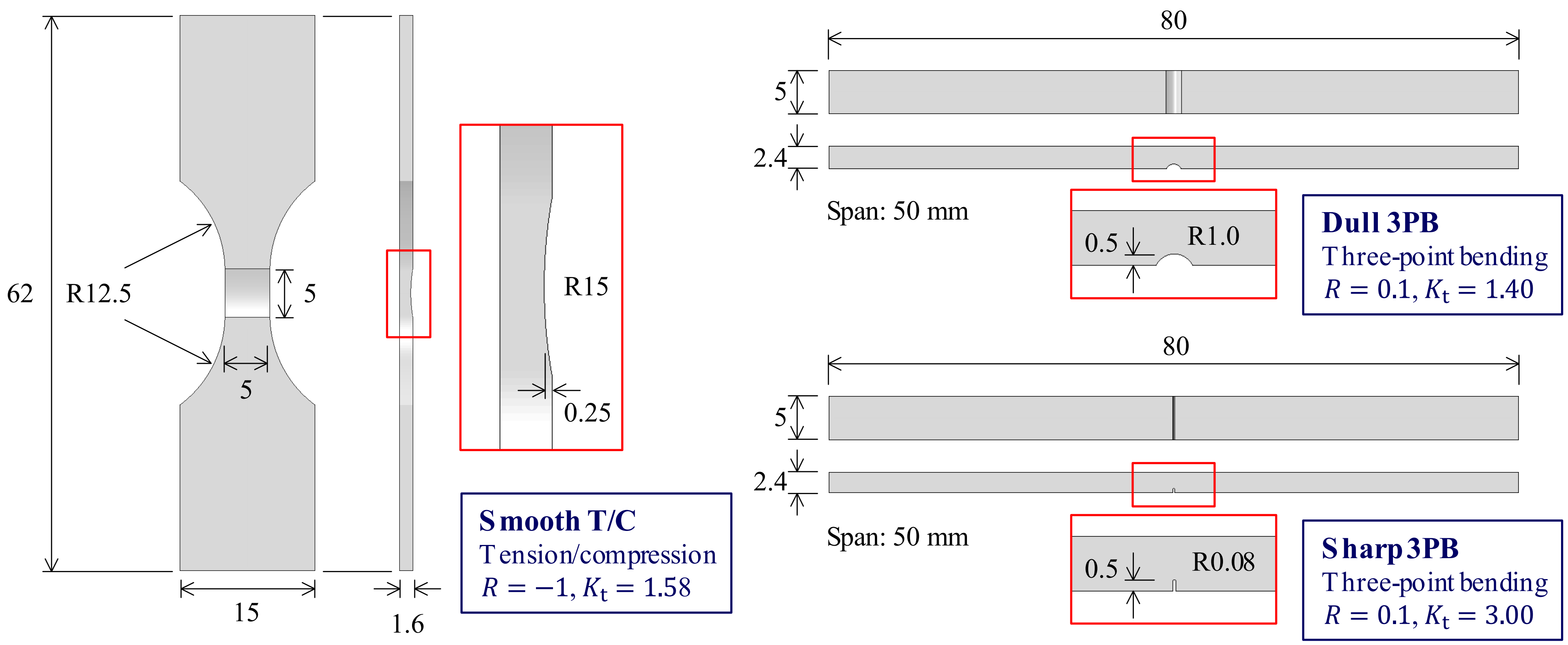
Chemical compositions [mass%]

Steel	C	Si	Mn	P	S	Al	N
A	0.18	0.15	1.00	< 0.002	0.0005	0.019	0.0008
B	0.087	0.15	1.00	< 0.002	0.0005	0.019	0.0008
C	0.14	0.36	1.54	0.014	0.002	-	-

Monotonic tensile properties and friction strength

Steel	Yield strength [MPa]	Tensile strength [MPa]	Reduction in area [-]	Ave. grain size [μm]	Volume fraction of pearlite [%]
A	216	430	0.72	56.6	27
B	260	395	0.79	24.5	13
C	368	538	0.78	15.4	21

Test conditions



- Three types of steels
- Three types of specimens

⇨ Nine types of fatigue tests

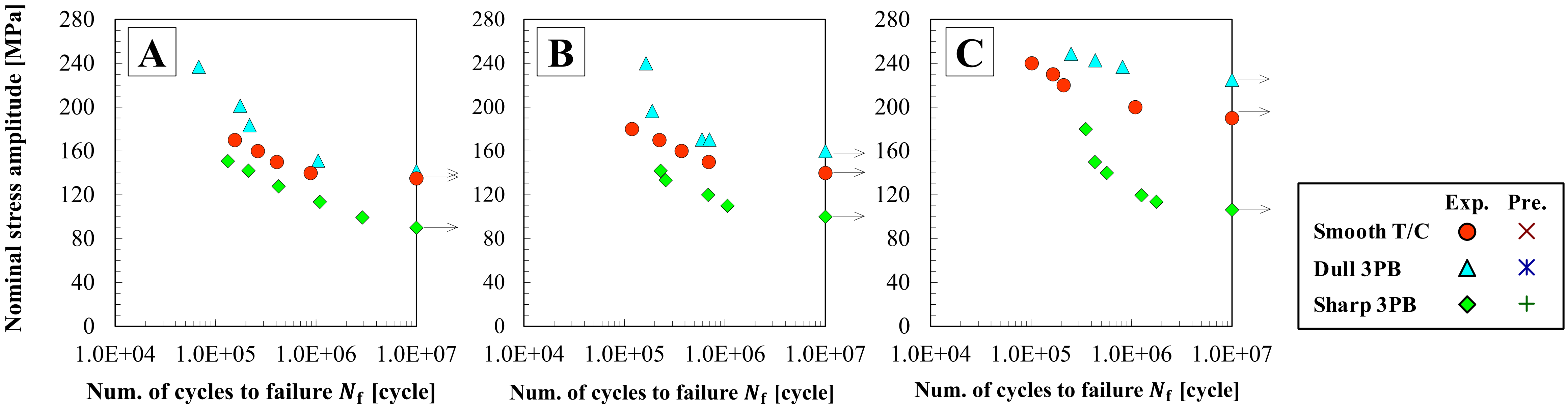
Prediction of S-N curves

Identification of constants in crack growth law:

$$\frac{da}{dN} = C(\Delta\mathrm{CTSD}^n - \Delta\mathrm{CTSD_{th}}^n)$$

Fitting for results of Smooth T/C of steel A

$C = 22.2,\ n = 2.0,\ \Delta\mathrm{CTSD_{th}} = 7.8 \times 10^{-2}\mu\mathrm{m}$



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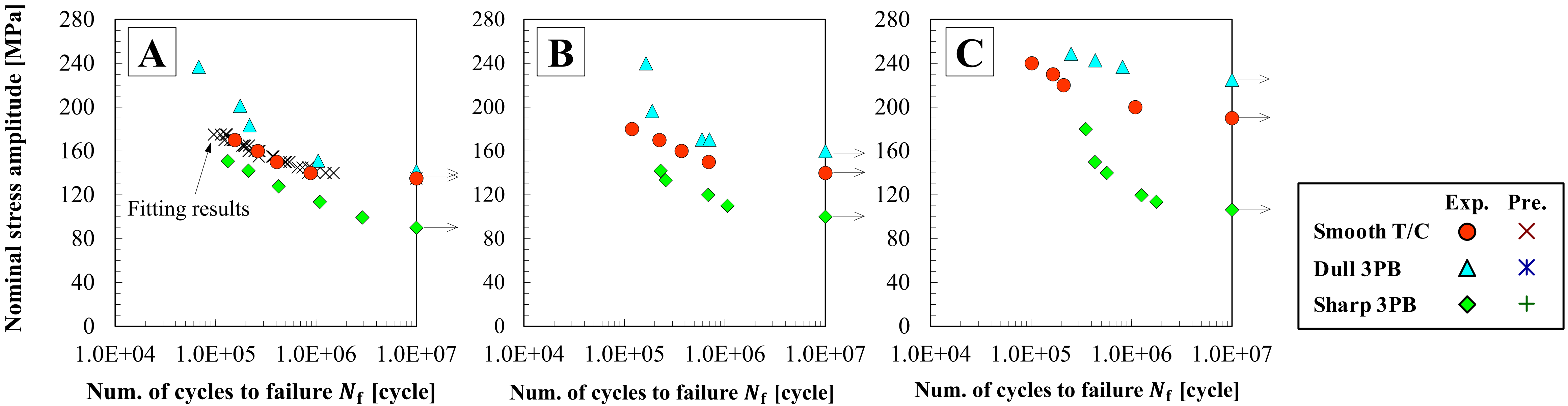

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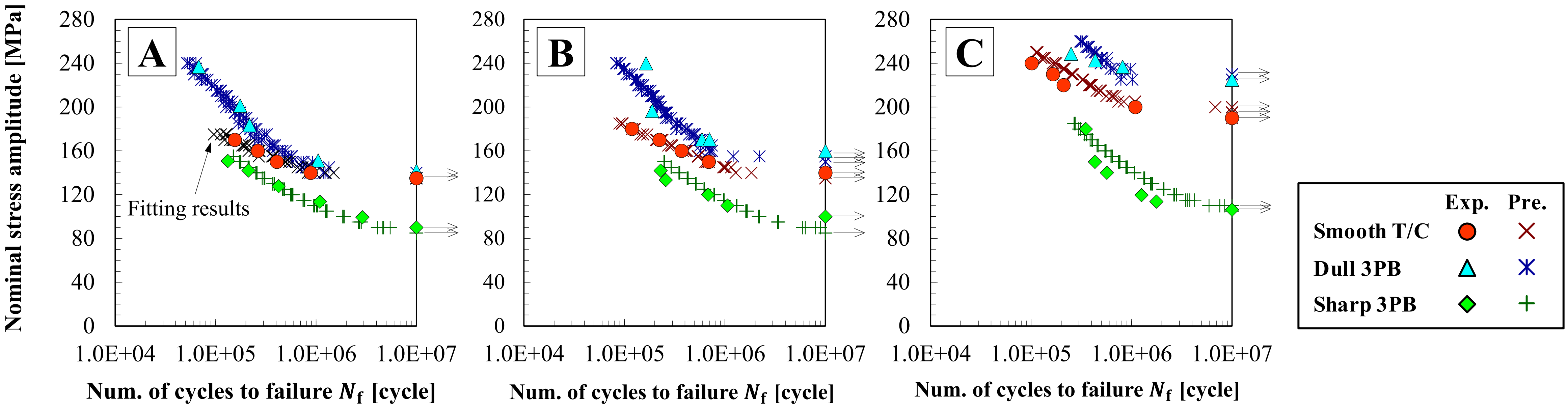

- Proposed model could successfully simulate all of experiments
- Fatigue life of steels can be predicted from crack growth life alone

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Summary

A model for predicting fatigue life and limit of steels

Experimental observation

- It was difficult to define crack initiation life in high cycle fatigue of steels.

Model development

- Prediction of fatigue life and limit based on microstructural information
- Total fatigue life calculated form crack growth life alone
- Reducing the dimension of problem as a 2D problem with 2 steps
- Multiscale model synthesis of three sub-models

Model validation

- Experiments using three types of steels and three types of specimen
- Fatigue lives and limits were successfully predicted.
- Fatigue life could be predicted from crack growth life alone.

References

K. Shibanuma*, K. Ueda, H. Ito, Y. Nemoto, M. Kinefuchi, K. Suzuki, M. Enoki
Materials and Design 139 (2018), 269-282.
Model for predicting fatigue life and limit of steels based on micromechanics of small crack growth

H. Ito, Y. Suzuki, H. Nishikawa, M. Kinefuchi, M. Enoki, **K. Shibanuma***
Multiscale model prediction of ferritic steel fatigue strength based on microstructural information, tensile properties, and loading conditions (no adjustable material constants)
International Journal of Mechanical Sciences 170 (2020), 105339

H. Zhou, Z. Liu, M. Kinefuchi, **K. Shibanuma***
Multiscale modelling strategy for predicting fatigue lives and limits of steels based on a generalised evaluation method of grain boundaries effects
International Journal of Fatigue 158 (2022), 106749


Materials and Design
Model for predicting fatigue life and limit of steels based on micromechanics of small crack growth


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