Grain Refinement and Viscous Fracture of Metals during Severe Plastic Deformation: Mathematical Simulation

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One of the Main Questions:

How can we increase the intensity of grain refinement and decrease failure?

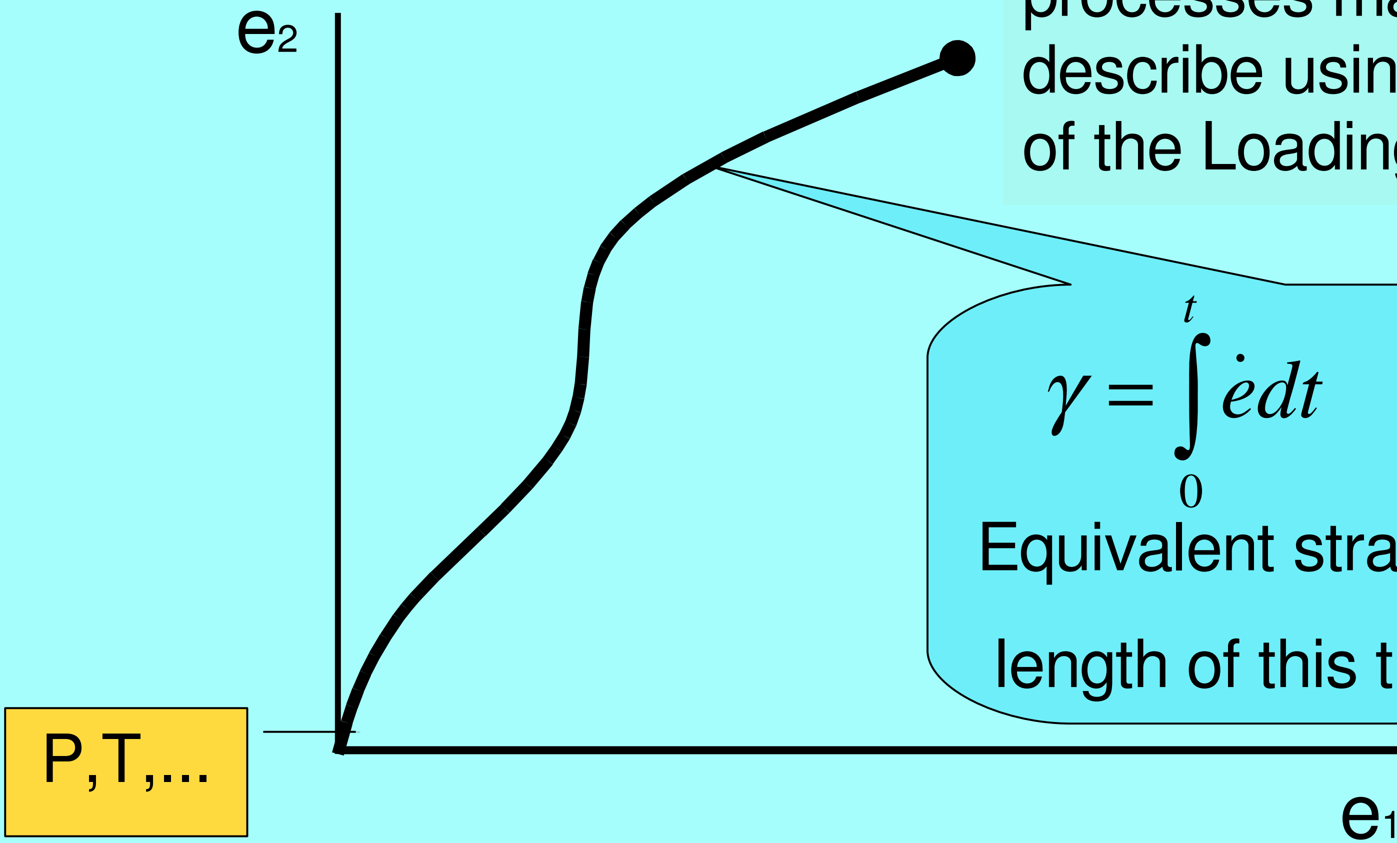
The Problem

One of the main problems faced by any approach is the multi-level character of the plastic deformation

Micro-macro interdependency

The Image of the Loading Process

In the mechanics of solids, any deformation processes may be describe using the image of the Loading processes

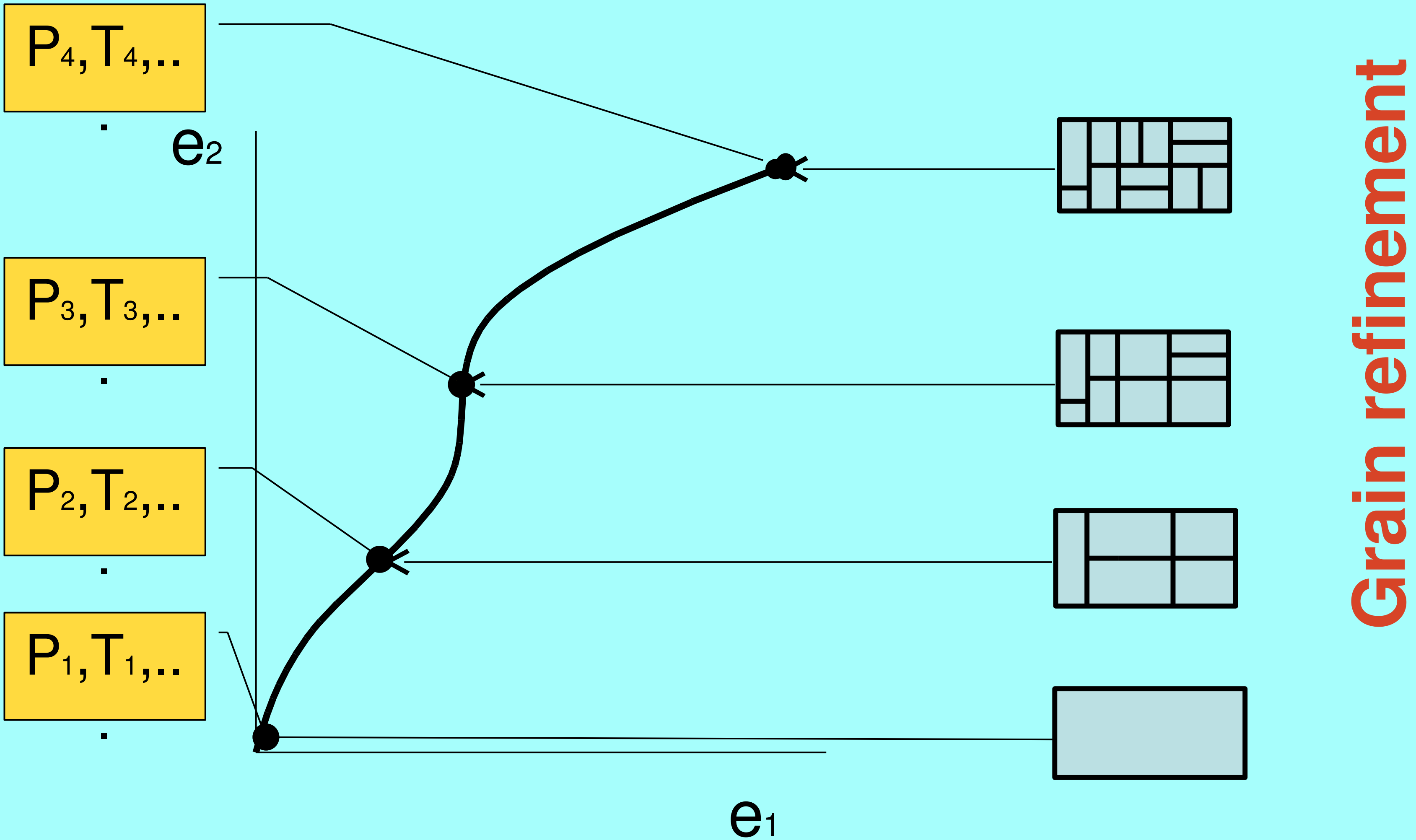


$$\gamma = \int_0^t \dot{e}\,dt$$

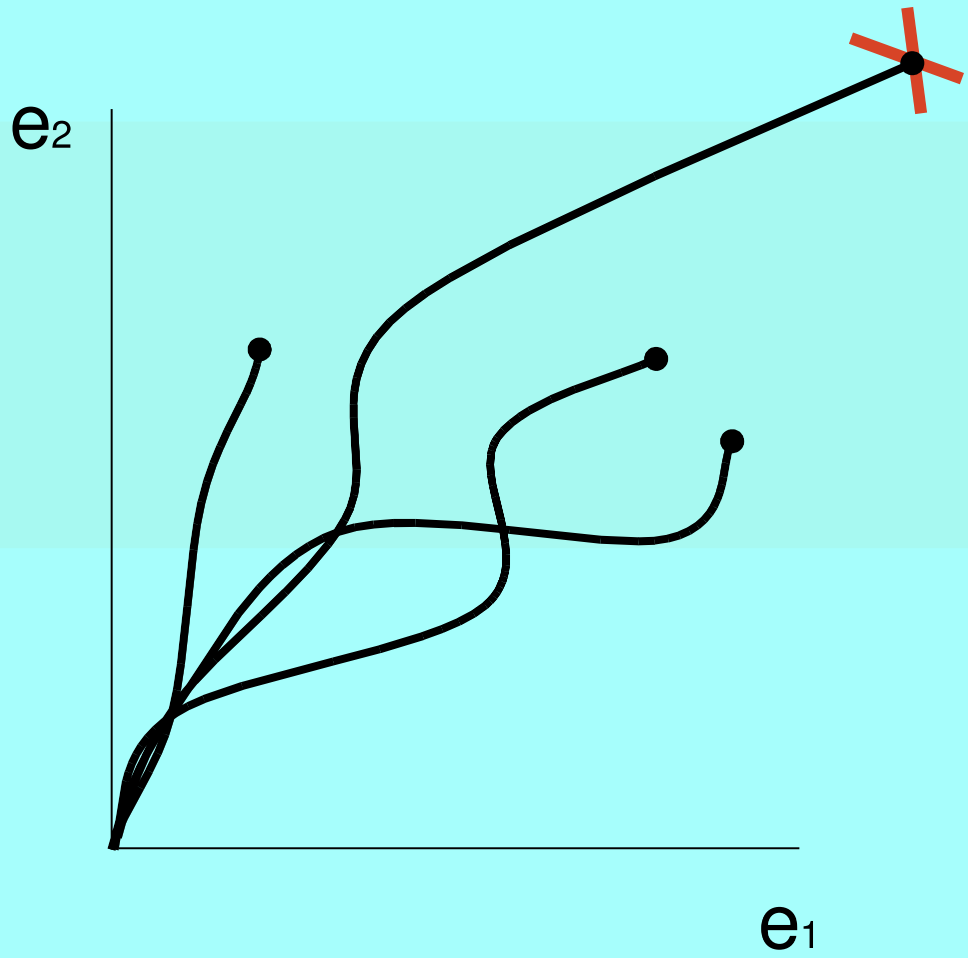
Equivalent strain =

length of this trajectory

Metal Structure is Determined by the Image of the Loading Process



But … The Image of The Loading Process depend on this structure



That is cause the dissipation of the loading paths for different materials points of the specimen

This is Interdependency

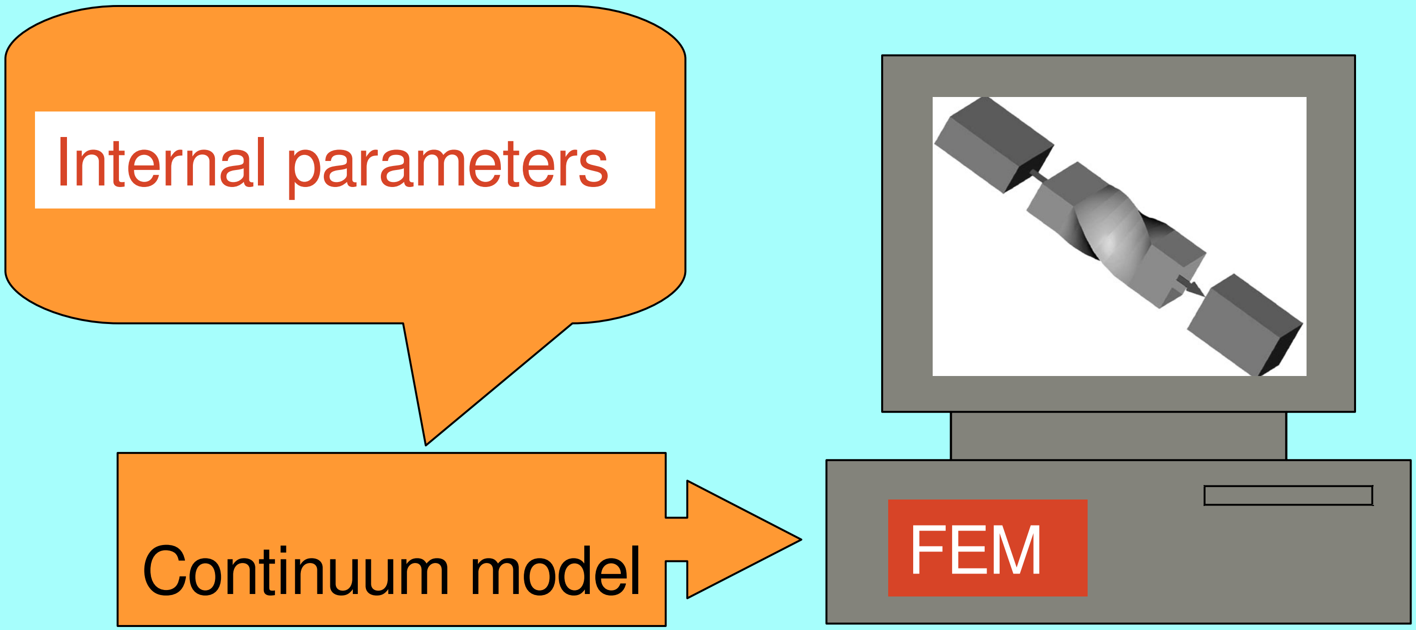
The Structure
of the Metal

The Image
of The Loading Process

The Problem

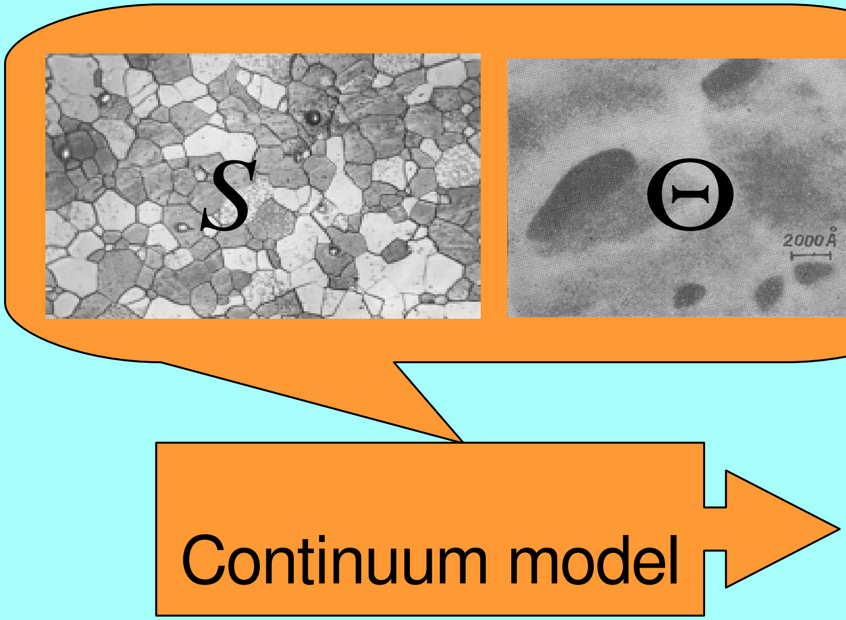
- We are trying to produce a given homogeneous structure in the volume of a specimen by deforming the specimen with a certain instrument. Moreover, we expect the metal to behave in a predictable way.
- In reality, however, the specimen may respond with a number of bad things: highly inhomogeneous structure, deformation localization, or fracture.
- The reason why this happens is precisely the **"Interdependency".**

Approach to describing interdependency



Internal parameters will allow us to account for the interdependency between the stress-strain state and the structure.

This talk

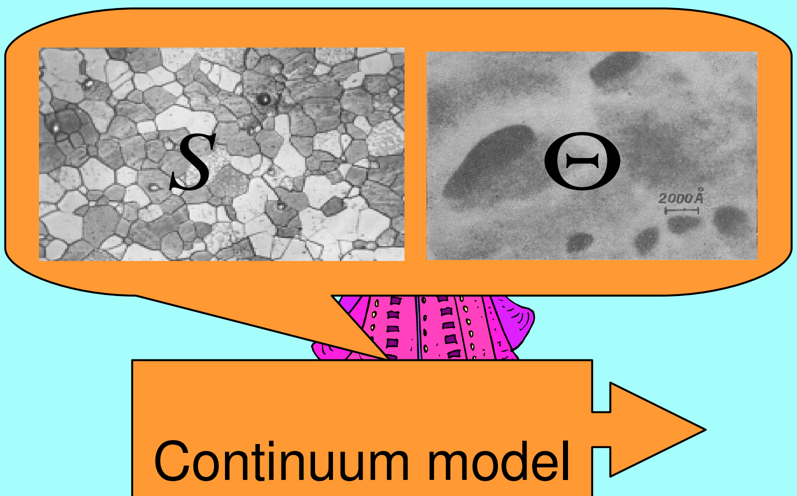


Continuum model describing two main interrelated processes co-existing in metals under SPD, namely grain refinement and fracture.

This talk

•***S*** - total length of the high-angle boundaries per unit of the cross section area

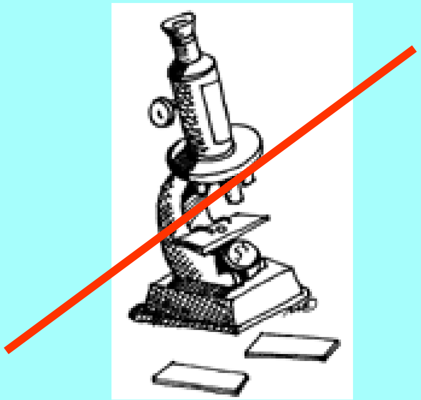
∀**Θ** - volume of micro-voids per unit volume of material.

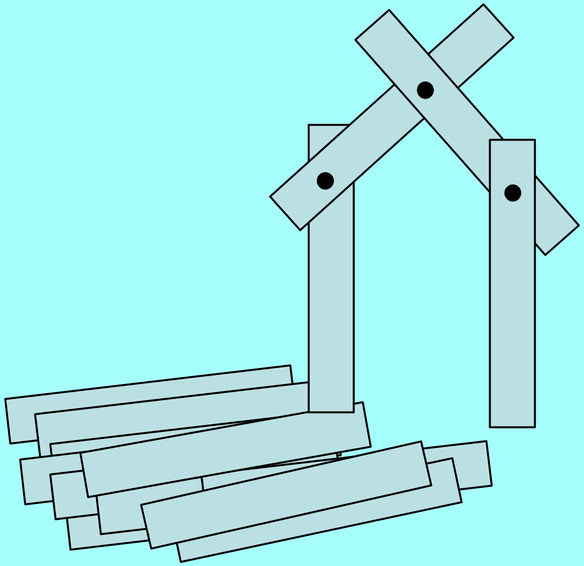


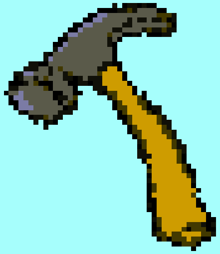
Internal parameters ***S*** and **Θ** should be considered as the special envoys representing the micro-level processes at the macro-level.

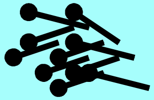
General remarks

- The model is based on several assumptions. This made the developed instrument much less precise than, for example, microscopes.
- On the other hand, this allowed us to make several consequences that may help to systematize the experiment.









General remarks

- Any model is a cartoon which emphasizes the characteristic features of the phenomenon. So I will use cartoons and simple mechanical models in my talk. I will introduce three characters which will help me to explain physical premises of the model.

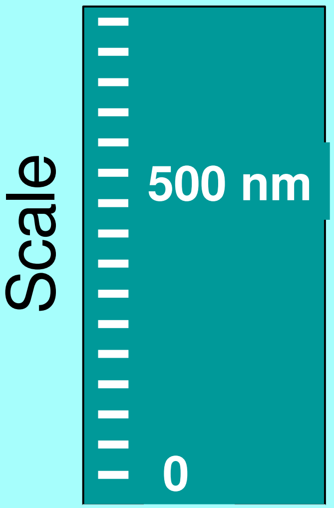
- In this talk I will present only main assumptions and consequences of the model. For more details see:

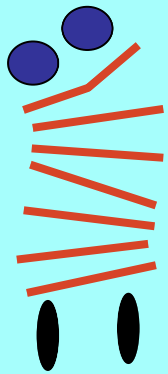
Beygelzimer Y. Grain Refinement Versus Voids Accumulation During Severe Plastic Deformation of Polycrystal: Mathematical Simulation
Mechanics of Materials , 2004 (in press)

Outline

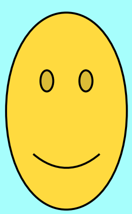
- Main characters
    - Birth
        - Life
            - Death
- The commandments
- Prediction

Main characters

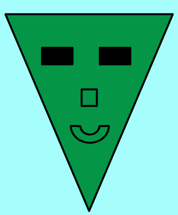




- **Accumulative Zone - **“spring”, part of crystals in which dislocation charges accumulate during plastic deformation; AZ emerge due to the inhomogeneity of shear along the sliding plane.



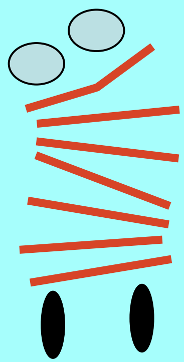
- **Void –** bit of an emptiness

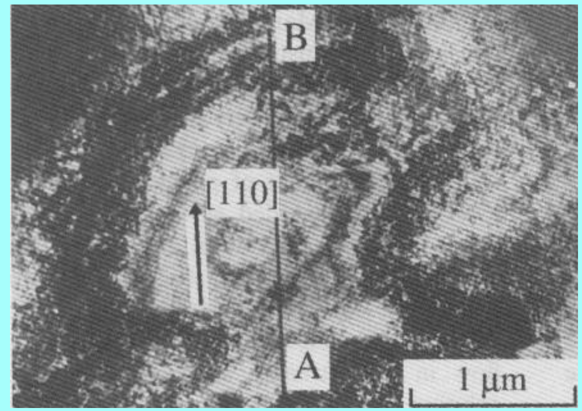


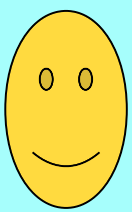
- **Embryo -** embryo of the high-angle boundary (partial disclination)

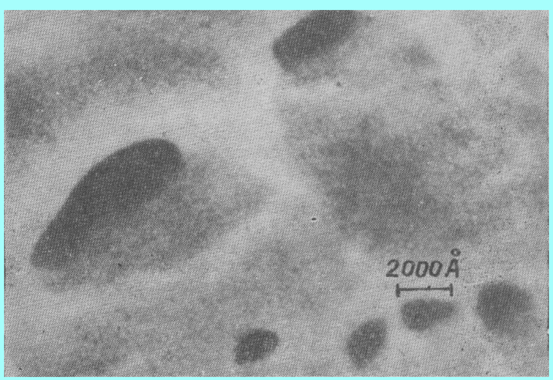
Pictures of Main characters

(A. Korotaev et al., 2001)

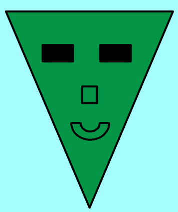








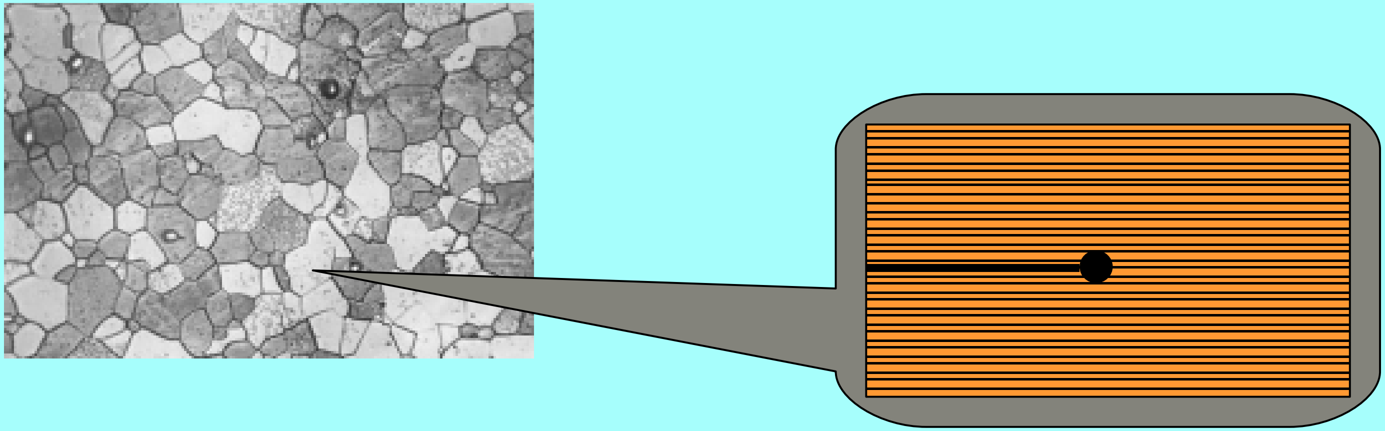
(V.Rubin, 1986)



(V.Betechtin et al., 1979)

Birth

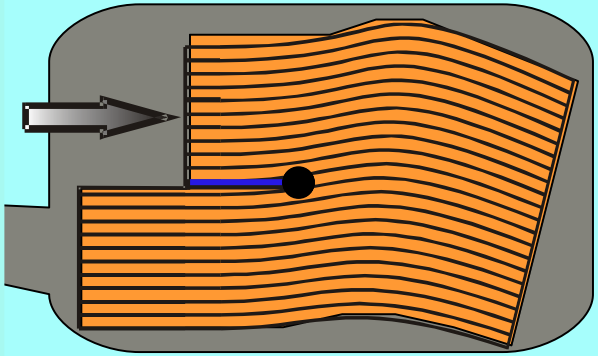
The Birth of Accumulative Zone

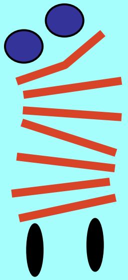


There are regions of polycrystal where dislocations get plugged during plastic deformation. Such regions cause bendings of the crystalline lattice.

The Birth of an Accumulative Zone

The model postulates that Accumulative Zones emerge in places of hurdles (e.g., grain boundaries) that exist in polycrystals before deformation, and also in high-angle boundaries that emerge during deformation.

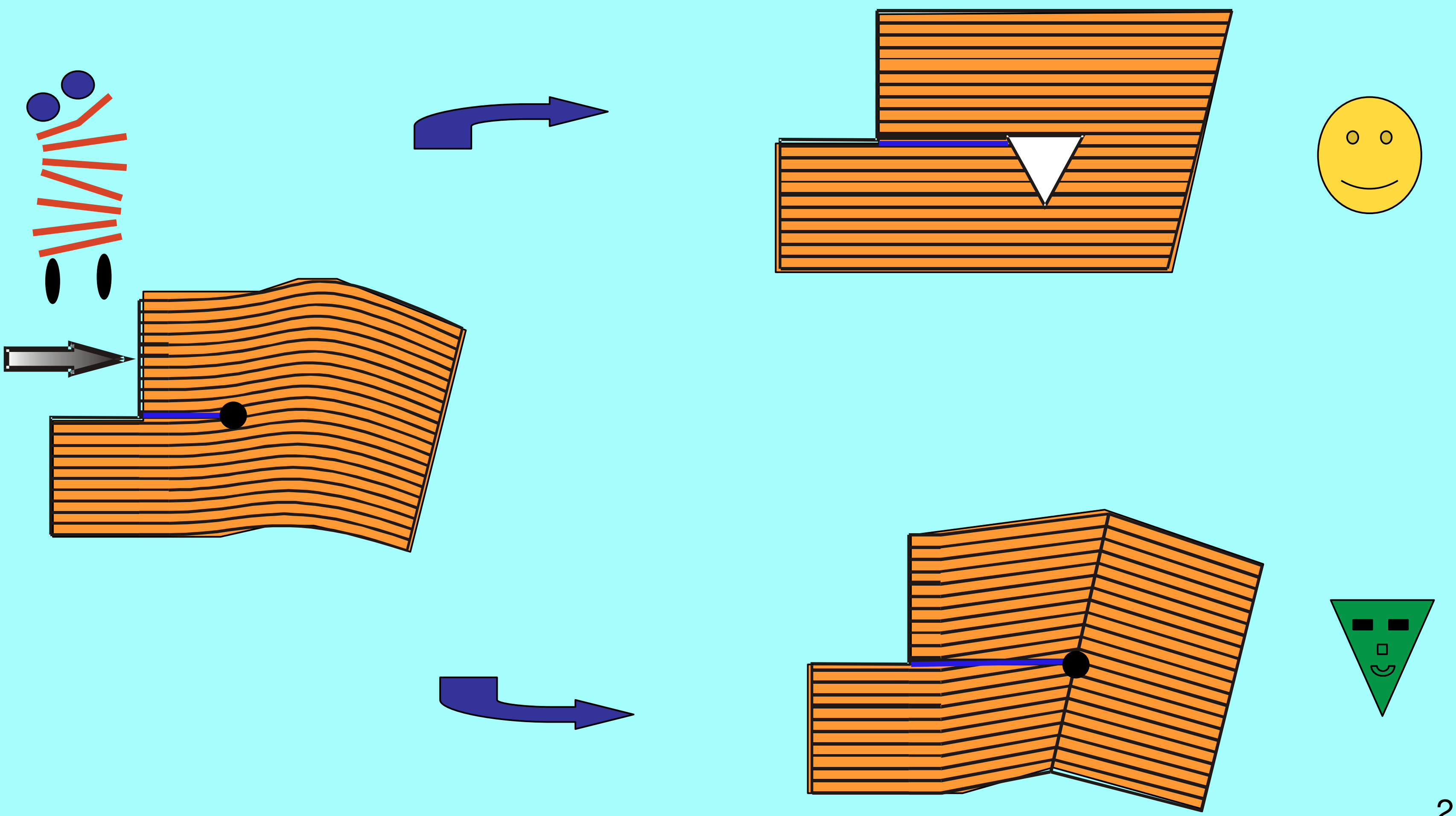




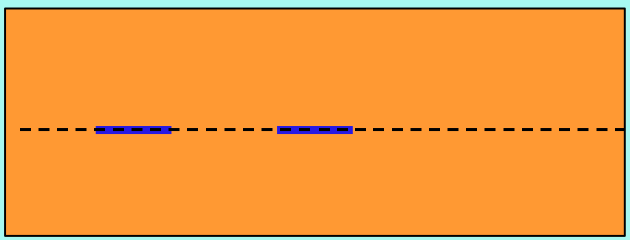
The Birth of a Void and an Embryo: Relaxations of Accumulative Zones.

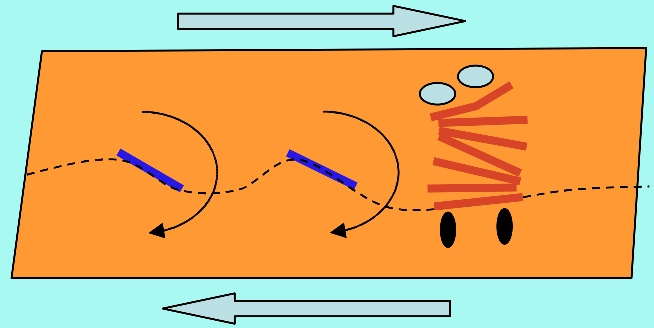
There are various relaxation mechanisms. When talking about large deformations, we will distinguish two main mechanisms: emergence of high angle boundaries and emergence of voids. The first mechanism leads to grain refinement, the second mechanism leads to fracture.

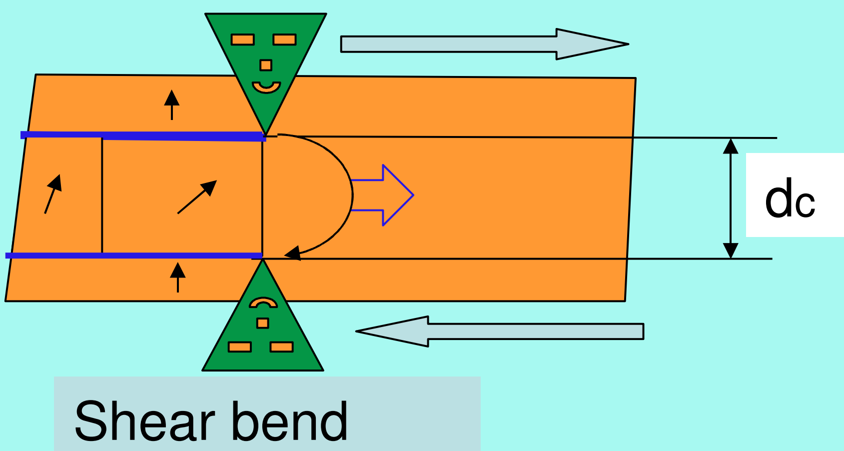
The Birth of a Void and an Embryo: Relaxations of Accumulative Zones.

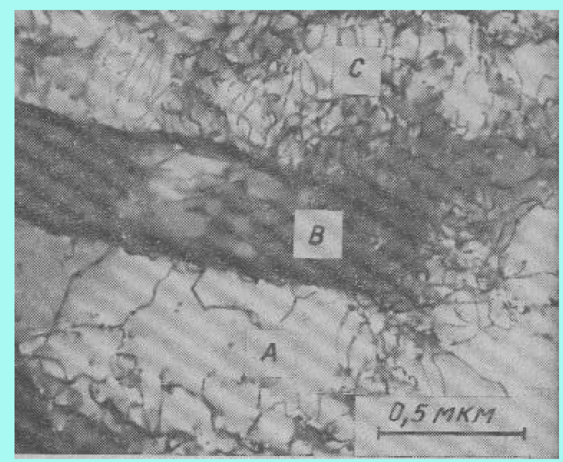


The Birth of a Couple of embryos



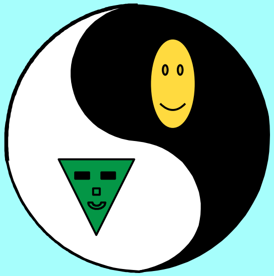


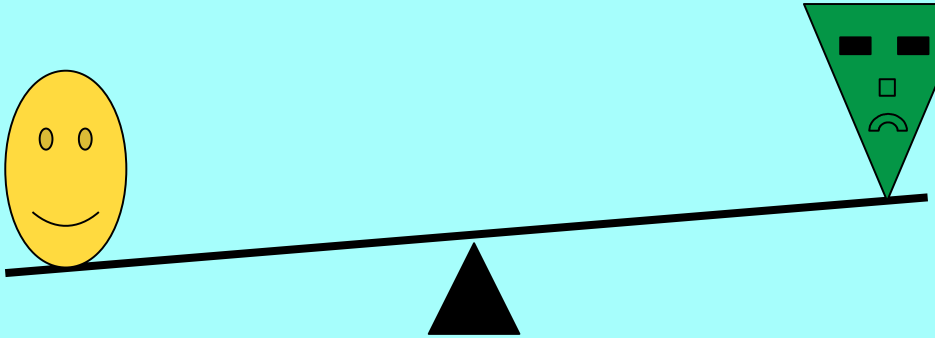




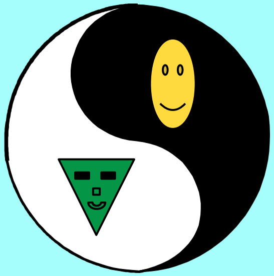
(V.Rubin, 1986)

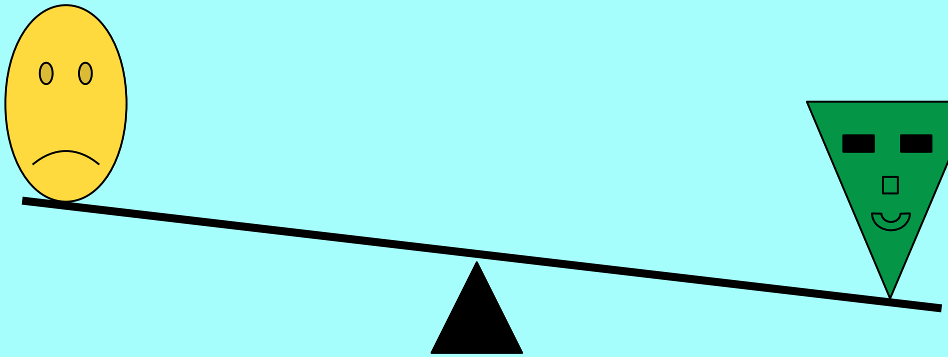
Assumption 1: complementarity of fracture and grain refinement





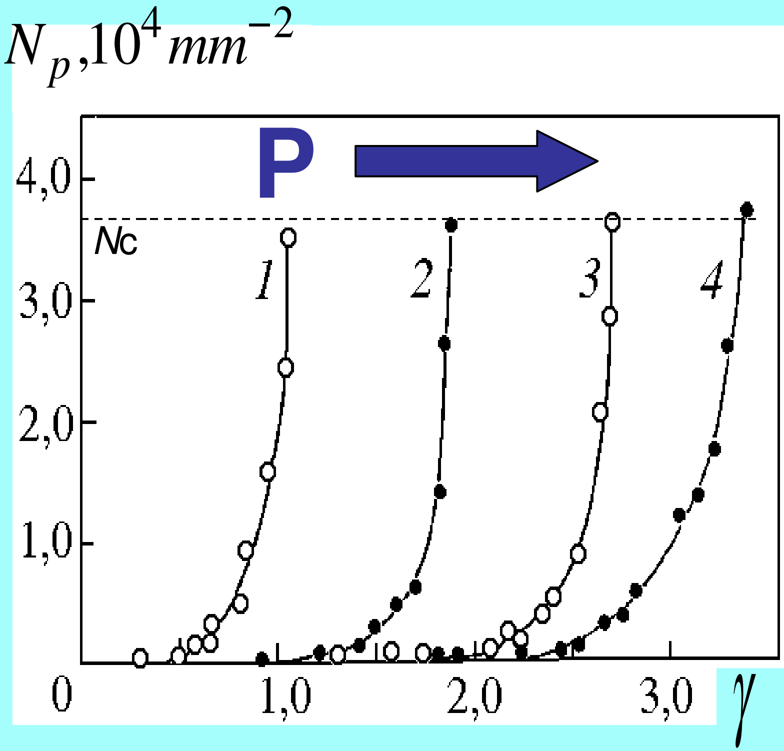
Assumption 1: complementarity of fracture and grain refinement





When one of them intensifies, the other subsides.

Hydrostatic Pressure Suppresses the Emergence of Voids

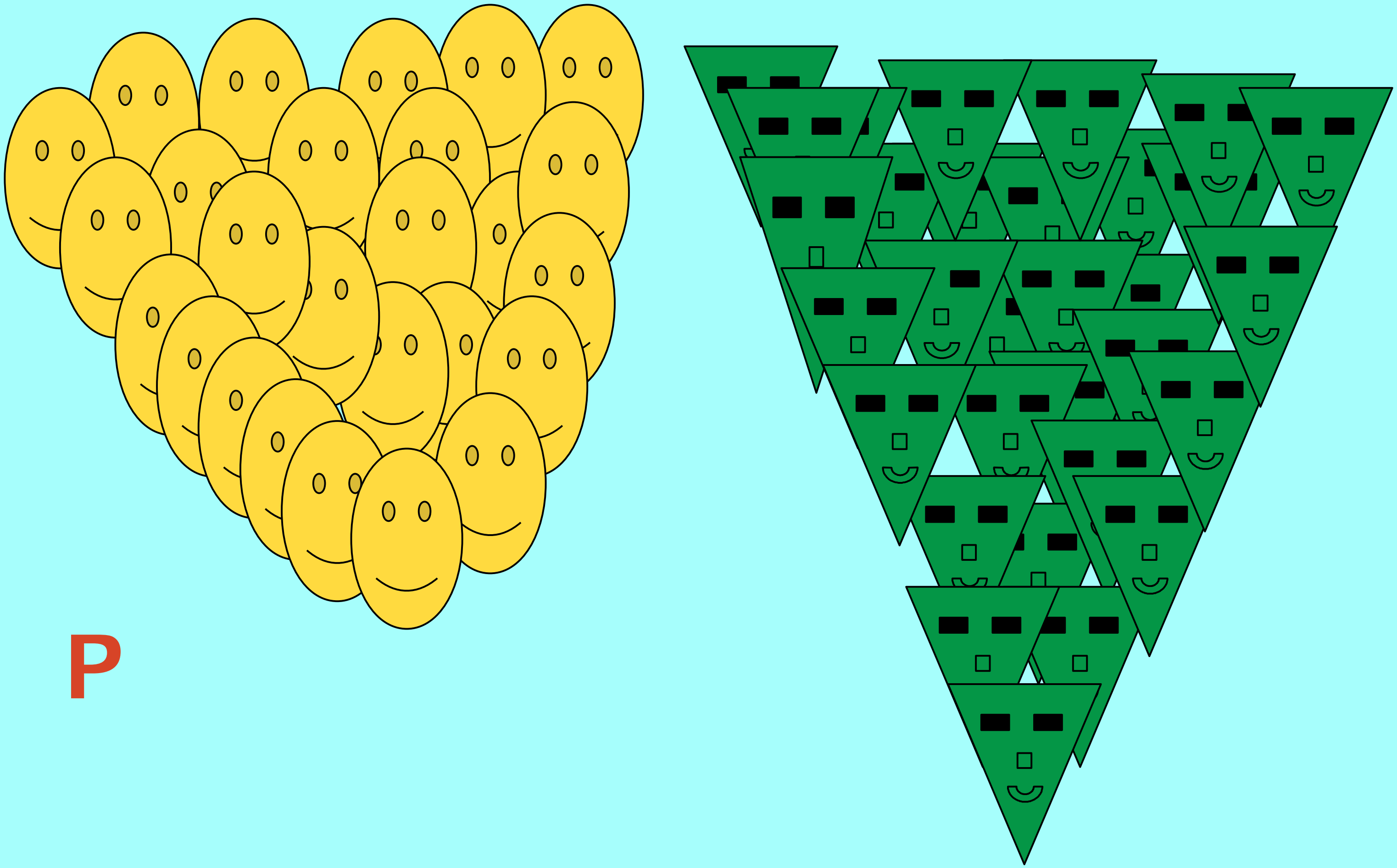


Uniaxial tension under pressure of a steel 1045 specimen (Kao A.S., et al., 1990); *N* - number of pores per unit square of specimen cross-section; γ - equivalent strain.

Hydrostatic pressure, MPa:

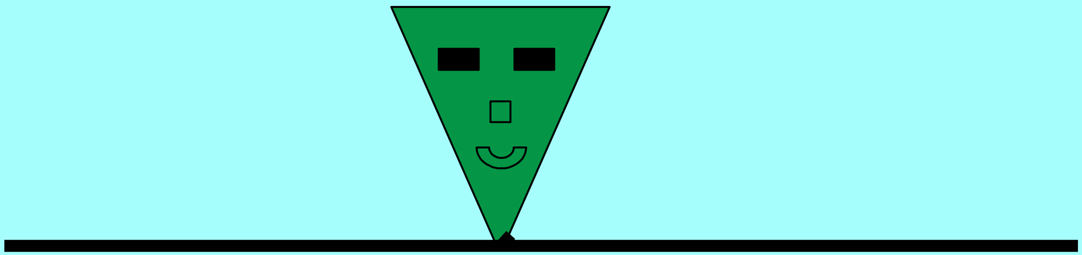
1- 0.1; 2- 420; 3- 840; 4 – 1120.

Complementarity implies that hydrostatic pressure intensifies the birth of Embryos of High Angle Boundaries



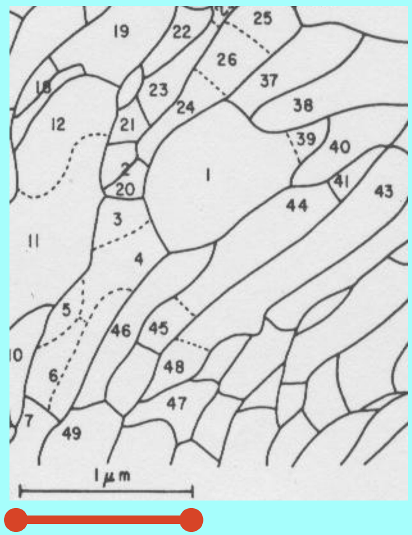
P

Life

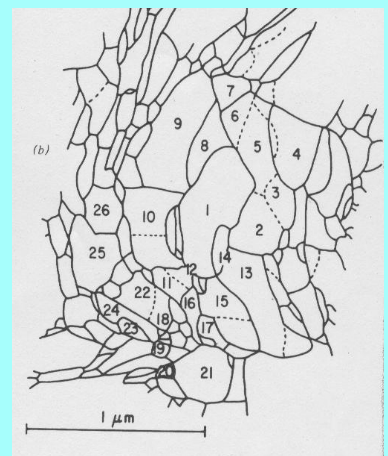


As strain increases, embryos move along the crystallites leaving traces in the form of high angle boundaries

This process results in grain refinement



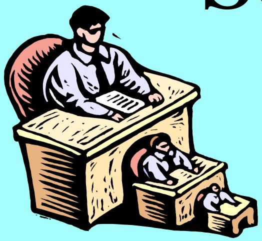
ε=2.5



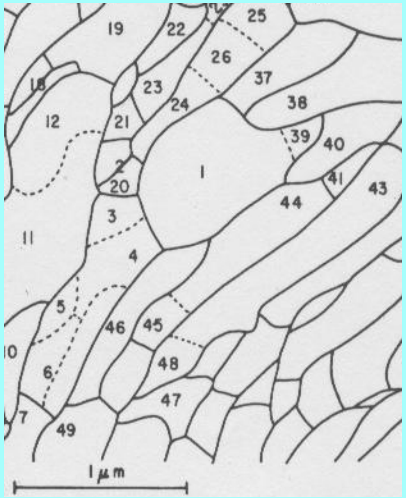
ε=5.8

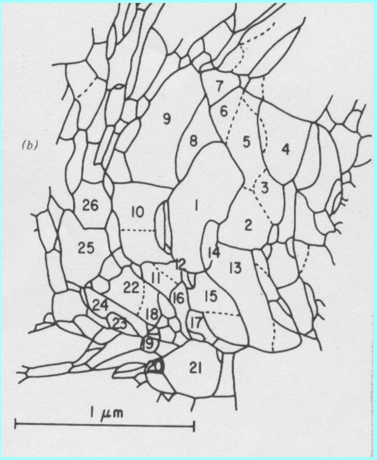
Fe, drawing (G.Langford and M.Cohen (1975))

Assumption 2:
Self-similarity of the grain refinement



Under certain conditions!





ε=2.5

ε=5.8

The structures obtained under different strain statistically differ only by their scale

Under what conditions can we expect self-similarity?

The answer is: When the mechanism of fragment division does not depend on the fragment size.

The same we can see at the various fragmentation processes.
For example on the glaze…

Under what conditions can we expect self-similarity?

or on the asphalt

When Fragment Division is Independent of Fragment Size?

We believe that this happens when

$$d_c << d << d_0$$

d_0 - average grain size

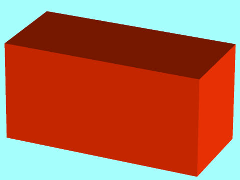
d_c - certain limiting size

What is d_c?

When the fragments become sufficiently small, they stop dividing. This is due to the fact that elastic stresses relax by fragment sliding along high-angle boundaries.

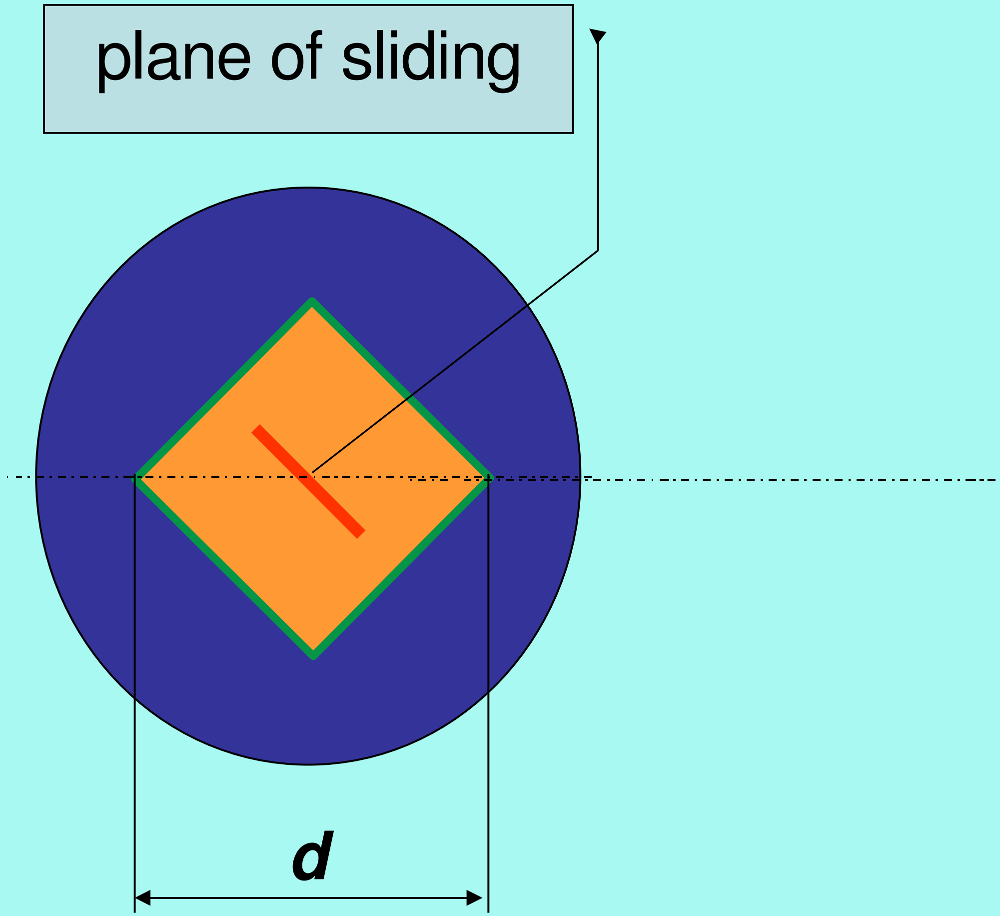
Assumption 3:

There is the limiting fragment size

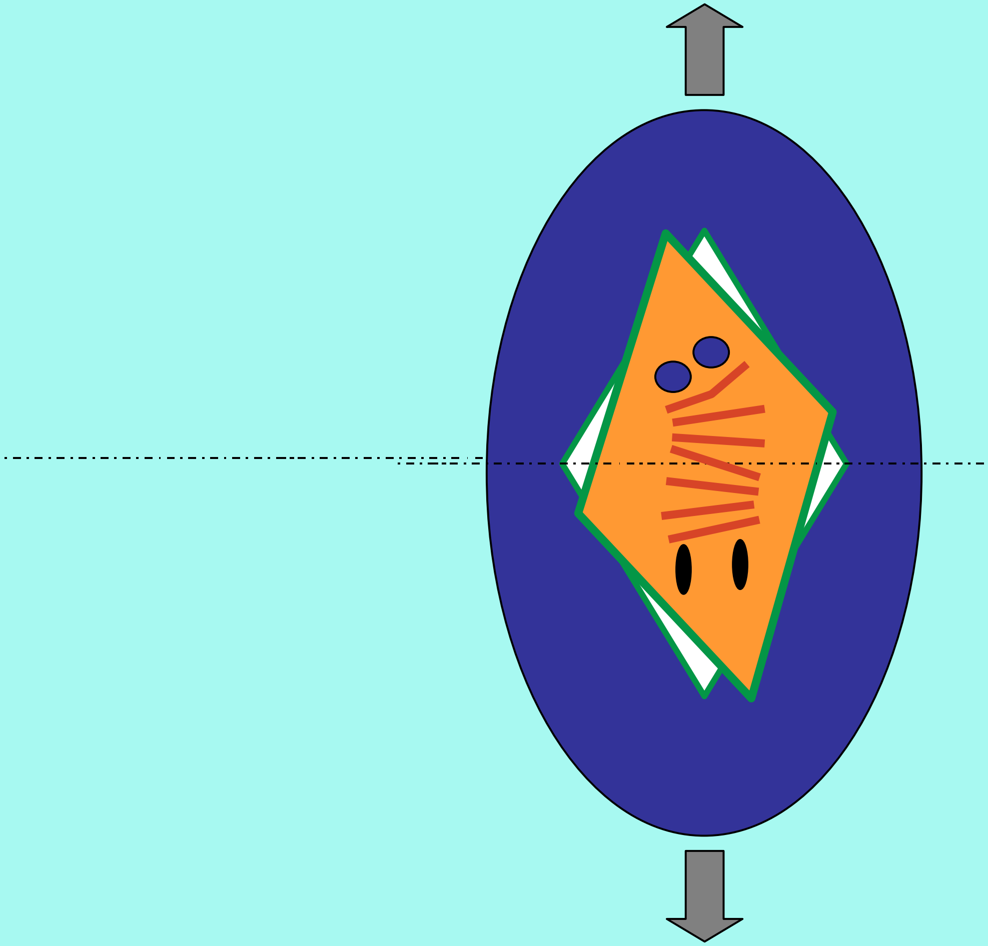


d_c Indivisible

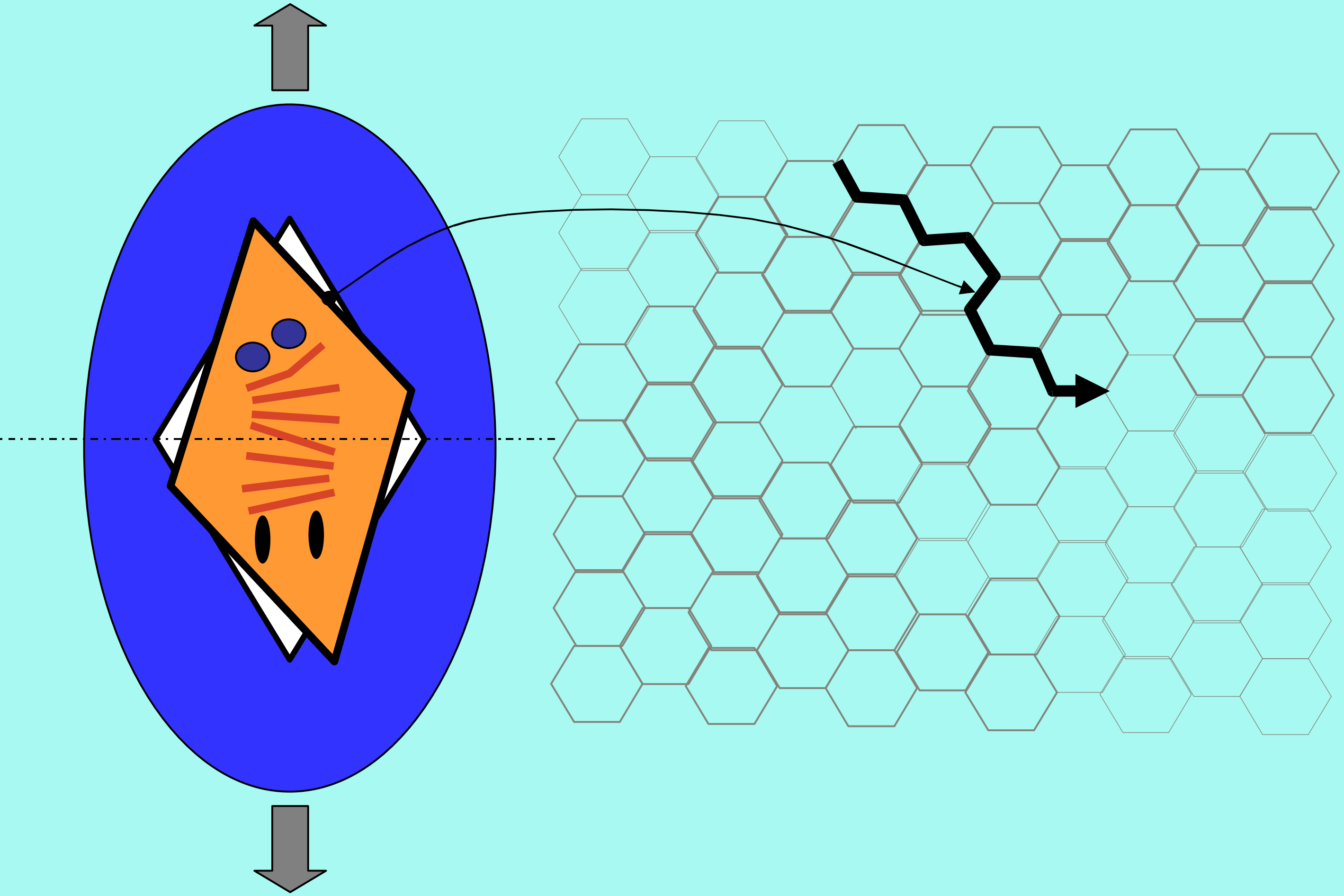
It happen when $d \rightarrow dc$



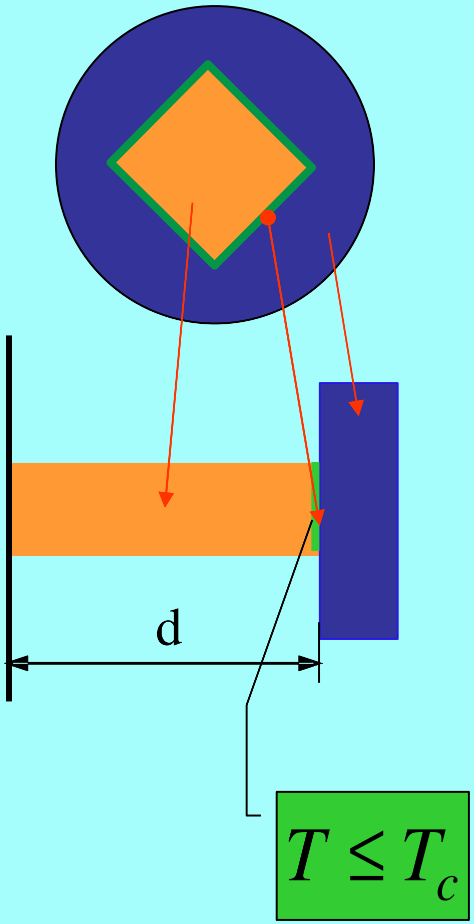
It happen when $d \to d$c



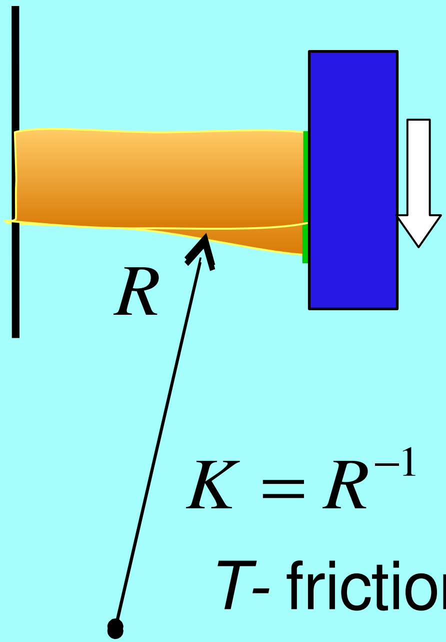
It happen when $d \rightarrow dc$



A Simple Mechanical Model explaining the existence of the limiting fragment size

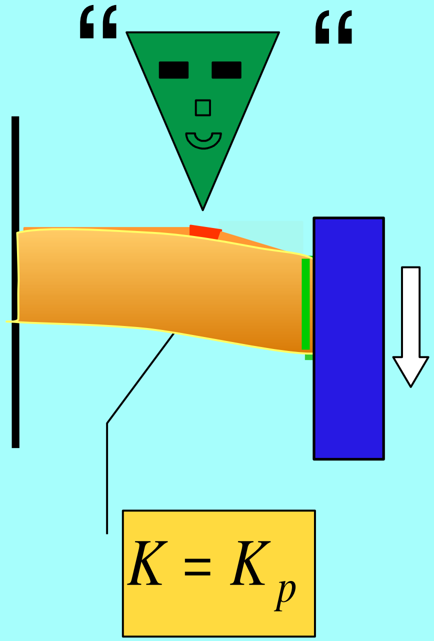


- Elastic beam represents a fragment.
- Fragment environment is represented by a slider pressed to the beam.
- There is friction with limiting value T_c between the slider and the beam.



Movement of the slider bends the beam. The curvature of the beam is related to the friction force via the following equation:

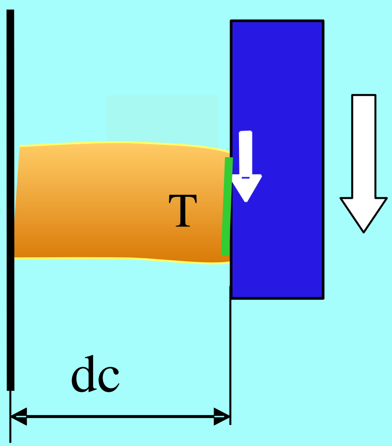
$$K = \frac{M}{J} = \frac{Td}{J}$$



- When the bending reaches a critical curvature $\boldsymbol{K}_p$, a plastic zone emerges.

- This leads to a decrease of elastic energy, and the bending transforms into a disorientation boundary.

- This boundary is an analog of a high-angle boundary



•Because the friction has the limit if the beam length is small we can't to bend the beam to the curvature K_p.

•Plastic zones can’t appear in such short beams, thus there can be no disorientation boundaries.

Plastic zones can appear only when the following condition is satisfied:

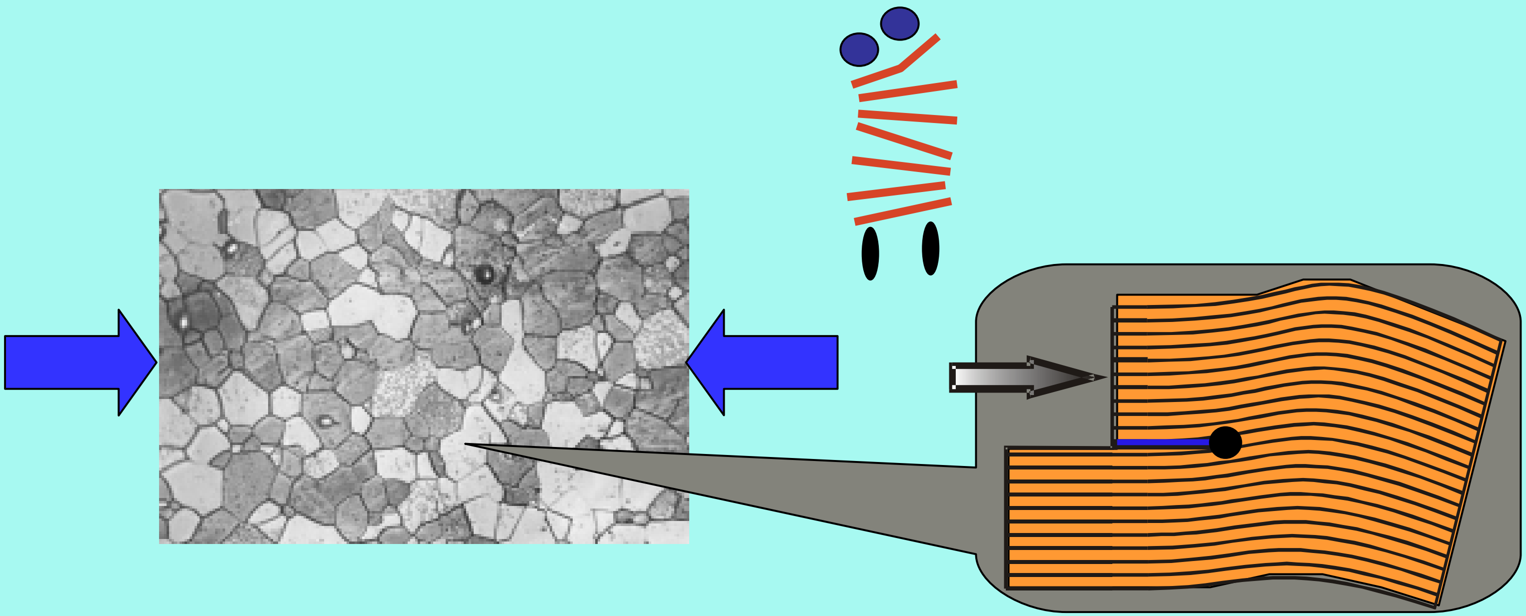
$$d \geq d_c = \frac{K_p J}{T_c}$$

J – stiffness of the beam

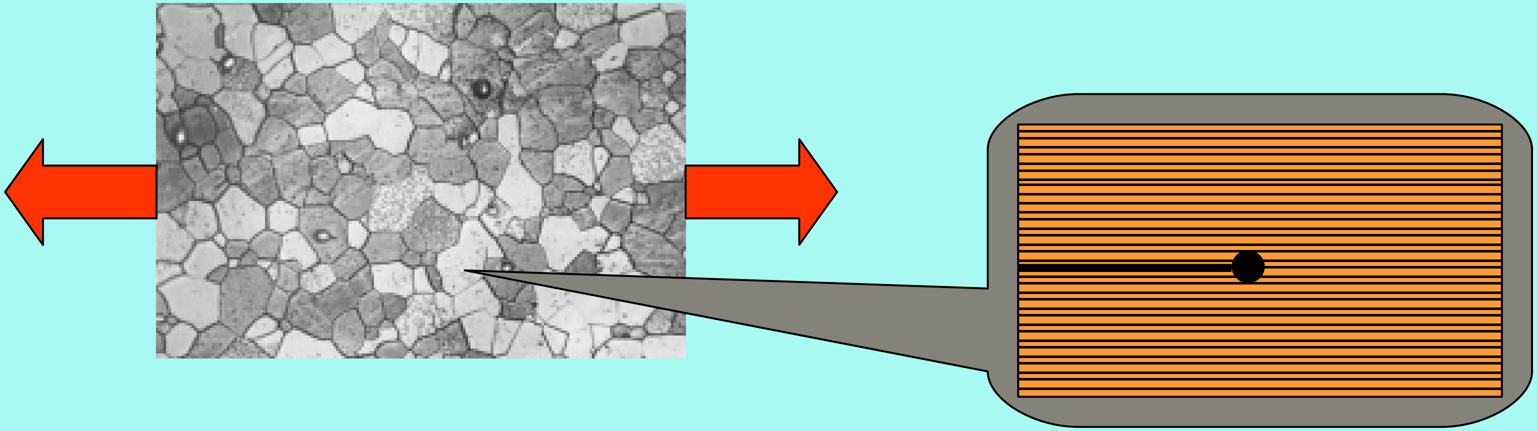
It is not proof, but this is plausible reasoning!

Death

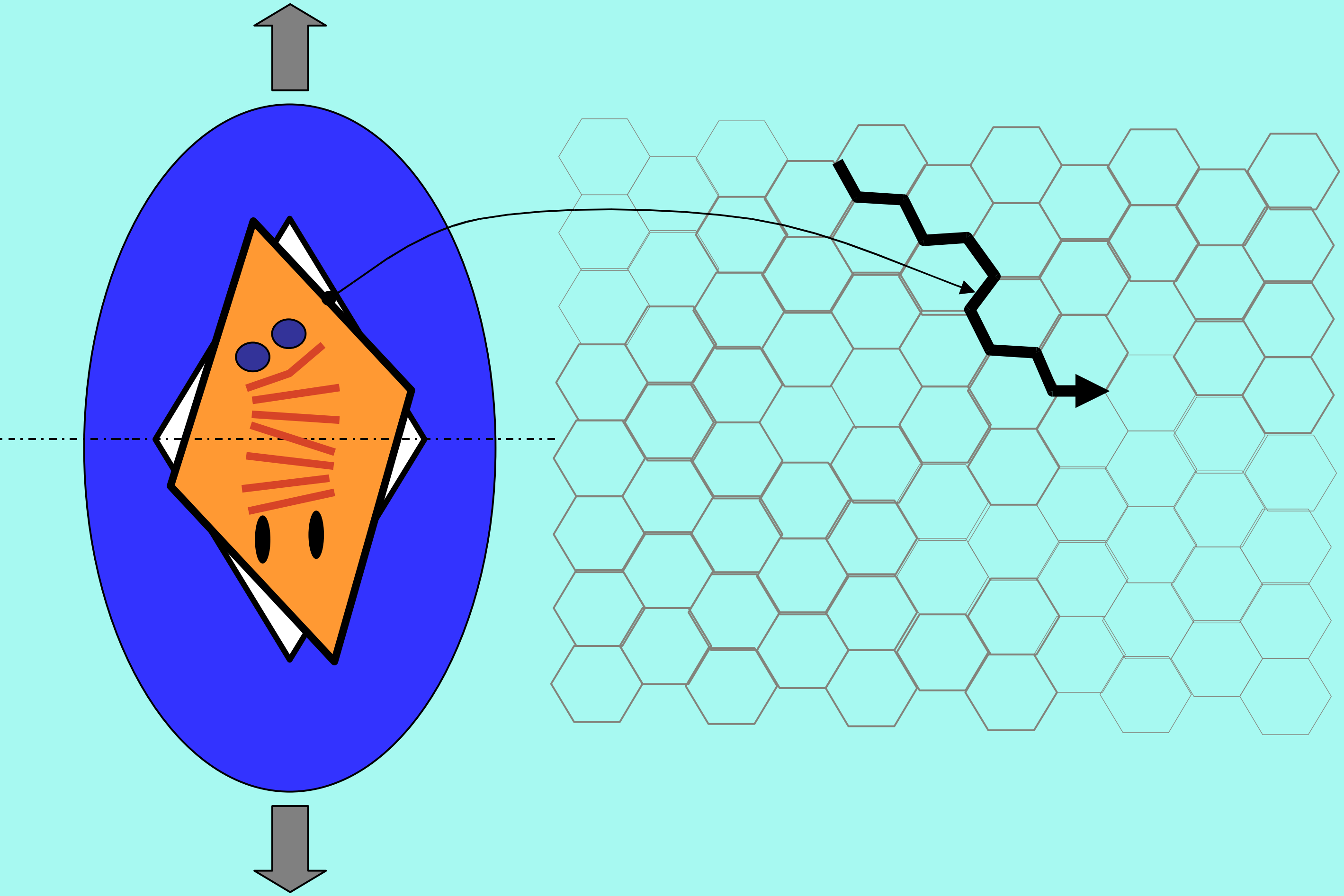
The Death of an Accumulative Zone During the Reverse Loading



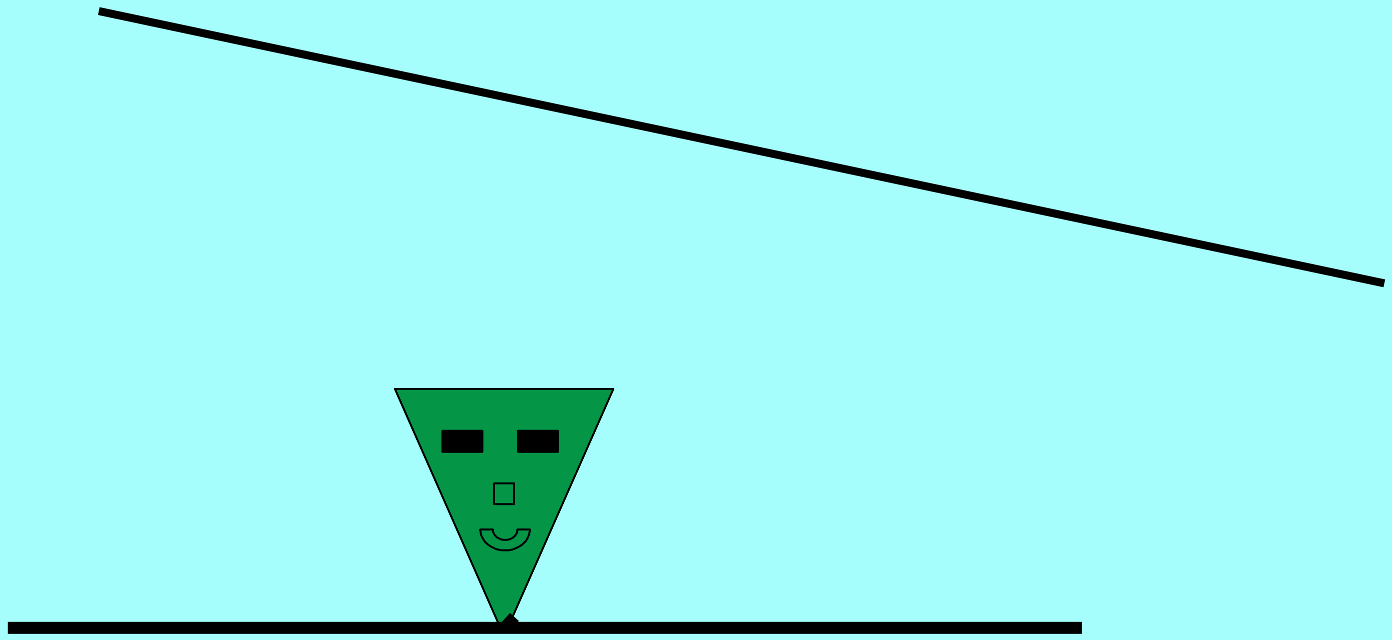
The Death of an Accumulative Zone During the Reverse Loading



The death of AZ related with sliding along the high angle boundary

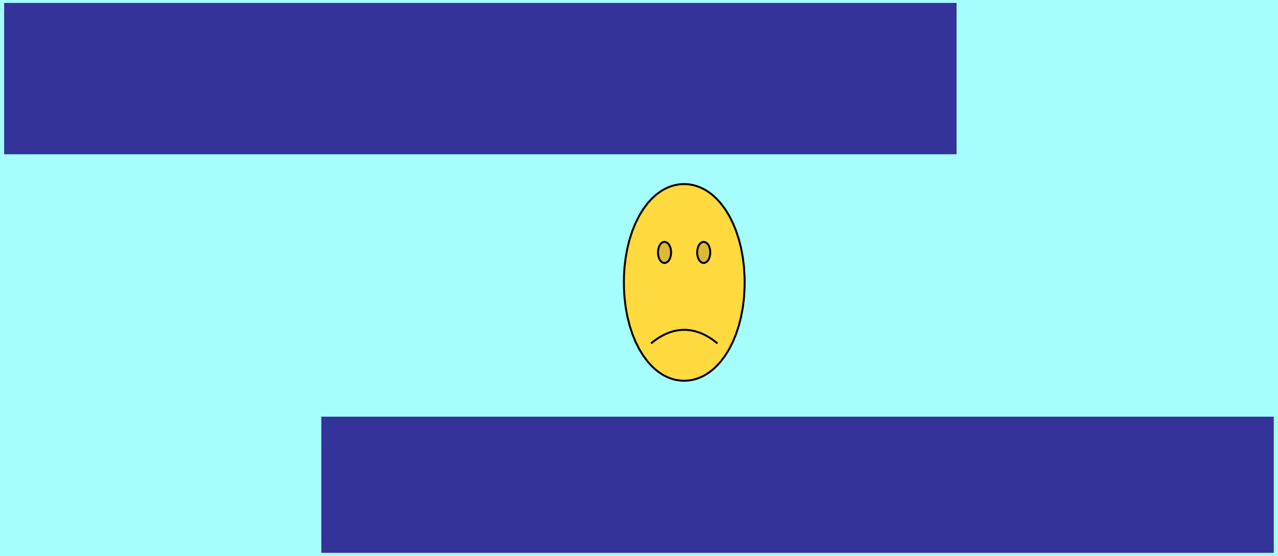


The Death of an Embryo of High-angle boundary



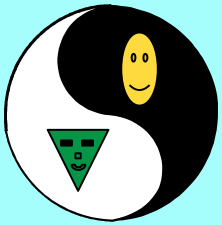
Embryos die when they reach a high-angle boundary. This happens because fragments can slide along these boundaries.

The Death of a Void

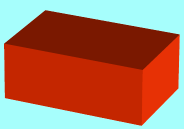


Voids die from shift deformations under pressure.
For a mathematical model explaining this effect see
Y.Beygelzimer et al., (1994) *Engin. Fracture Mech*., **48**, N5

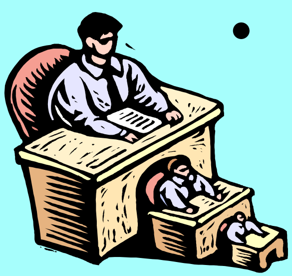
Main assumptions



- There are only two relaxation mechanisms of AZ: (1) the emergence of a void; (2) the emergence of an embryo of a high-angle boundary.



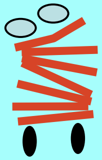
- There is a limiting fragment size d_c .



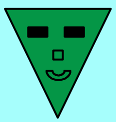
- When $d_c << d << d_0$, the mesh of high-angle boundaries develops in a self-similar fashion

The Commandments

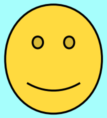
Table of symbols



- ***N*** - number of AZ per unit of the cross section area
- ***S*** - total length of the high-angle boundaries per unit of the cross section area



- N_b - number of embryo of the high-angle boundary per unit of the cross section area



- N_p - number of voids per unit of the cross section area
- Θ - porosity

Kinetic equations

Birth **Life** **Death**

$$
\begin{cases}
\dfrac{d\overline{N}}{d\gamma} = \left(C_1 + C_2 C_5 \overline{N}_b\right) F\left(\overline{S}\right) - \left(C_3 + C_4\right)\overline{N} \\
\dfrac{d\overline{N}_b}{d\gamma} = C_4 \overline{N} - C_5 \overline{N}_b \\
\dfrac{d\overline{S}}{d\gamma} = \dfrac{C_5 \overline{N}_b}{\overline{S} + \overline{S}_0} \\
\dfrac{d\Theta}{d\gamma} = C_3 \overline{N}^{\frac{3}{2}} d_c^{-3} v - C_6 \Theta
\end{cases}
$$

v -voids volume

$\overline{N} = 0 \quad \overline{N}_b = 0$

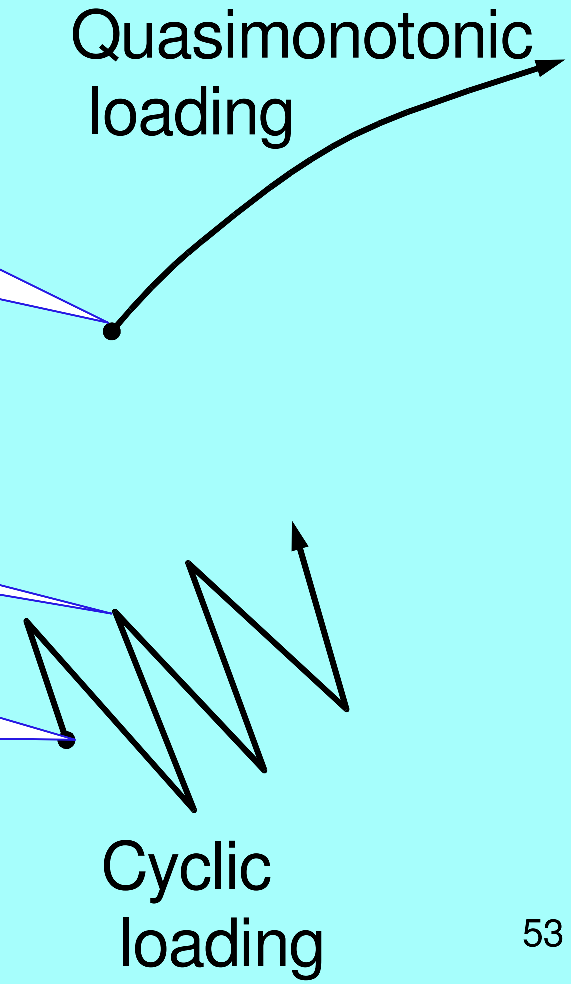
$\overline{S} = 0 \quad \Theta = 0$

$\overline{N}_{n+1} = 0 \quad \overline{N}_{b(n+1)} = \overline{N}_{b(n)}$

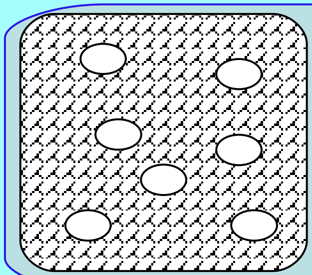
$\overline{S}_{n+1} = \overline{S}_n \quad \Theta_{n+1} = \Theta_n$

$\overline{N} = 0 \quad \overline{N}_b = 0$

$\overline{S} = 0 \quad \Theta = 0$



Constitutive equations



RVE- Porous body with structural framework

$$\begin{cases} f\left(\sigma_{ij}; S, \Theta\right) = 0 \\ \dot{e}_{ij} = \lambda \dfrac{\partial f\left(\sigma_{ij}; S, \Theta\right)}{\partial \sigma_{ij}}; \end{cases}$$

The principal relationships for the RVE

σ_{ij}, $\dot{e}_{ij}$ are the tensors of stresses and strain rates respectively

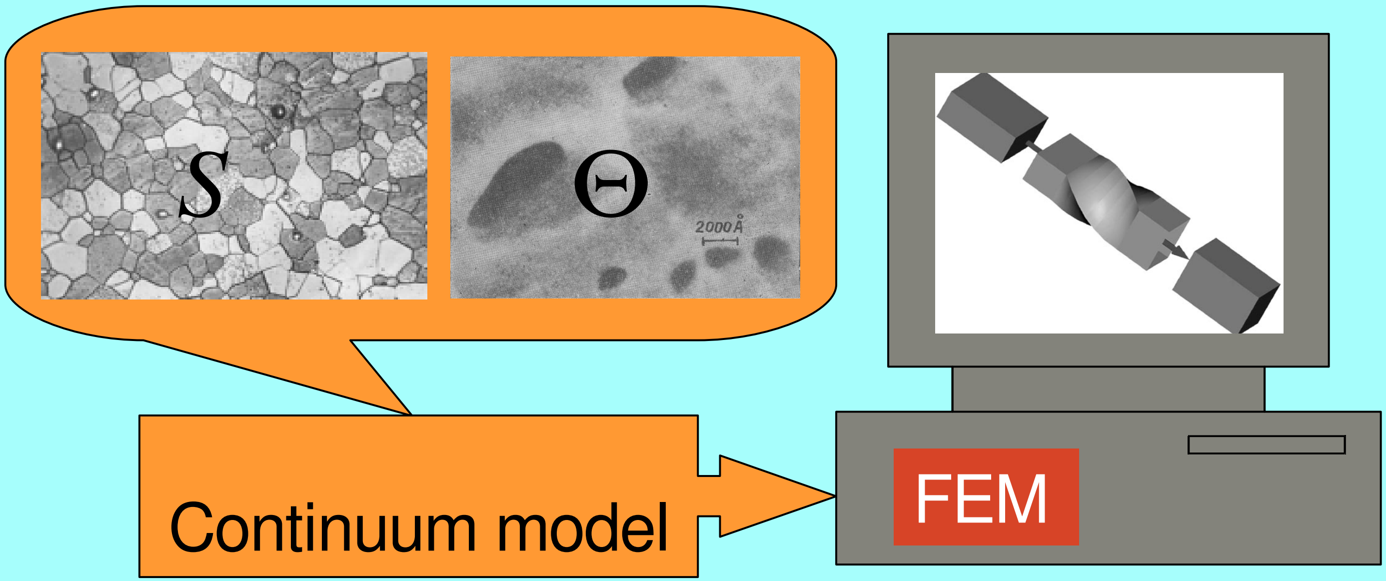
$$f\left(\sigma_{ij}; S, \Theta\right) = \frac{p^2}{\psi(\Theta)} + \frac{\tau^2}{\varphi(\Theta)} - (1-\Theta)\left(\frac{\sigma_s(S)}{\sqrt{3}} + \alpha^* p\right)^2$$

$$\tau = \sqrt{\left(\left(\sigma_{ik} + \frac{1}{3} p \delta_{ik}\right)\left(\sigma_{ik} + \frac{1}{3} p \delta_{ik}\right)\right)}$$

$$\alpha^* = C_3 \overline{N}^{\frac{3}{2}} d_c^{-3} v$$

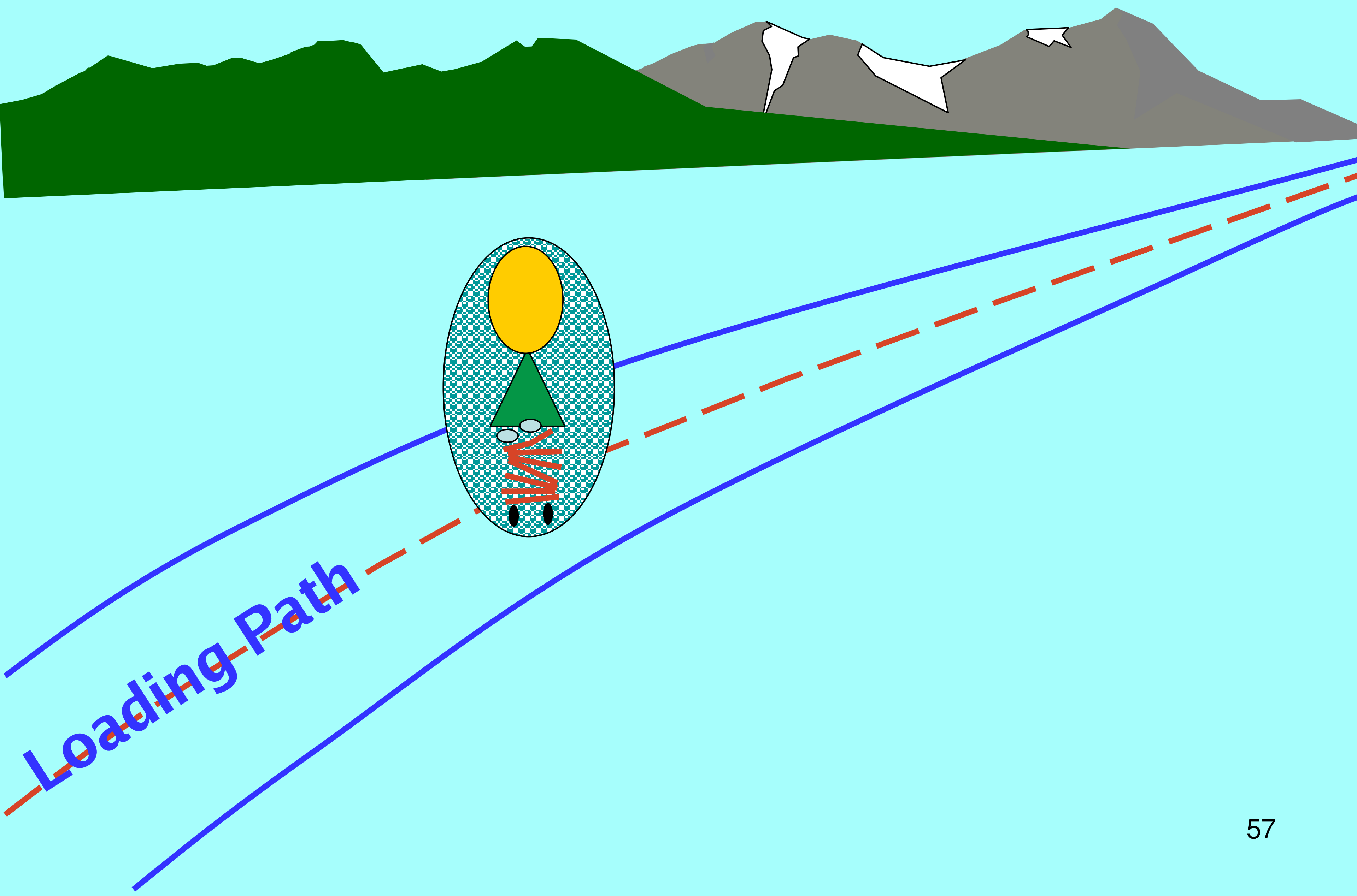
$$\psi(\Theta) = \frac{(1-\Theta)^{2n-1}}{6a\Theta^m}, \qquad \varphi(\Theta) = (1-\Theta)^{2n-1},$$

If one substitutes the Mises equations for these equations in any FEM package, one could directly compute the stress-state state of a metal and its dependence on the structure



Model parameters are obtained through compression and torsion tests

Prediction


Loading Path

(i)

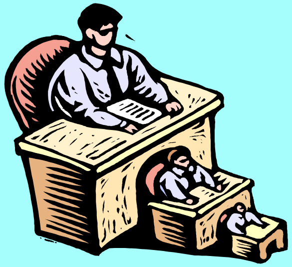
As $\gamma \to \infty$

$$N \to 0, \qquad N_b \to 0,$$

$$\bar{d} \to d_c, \qquad \Theta \to 0$$

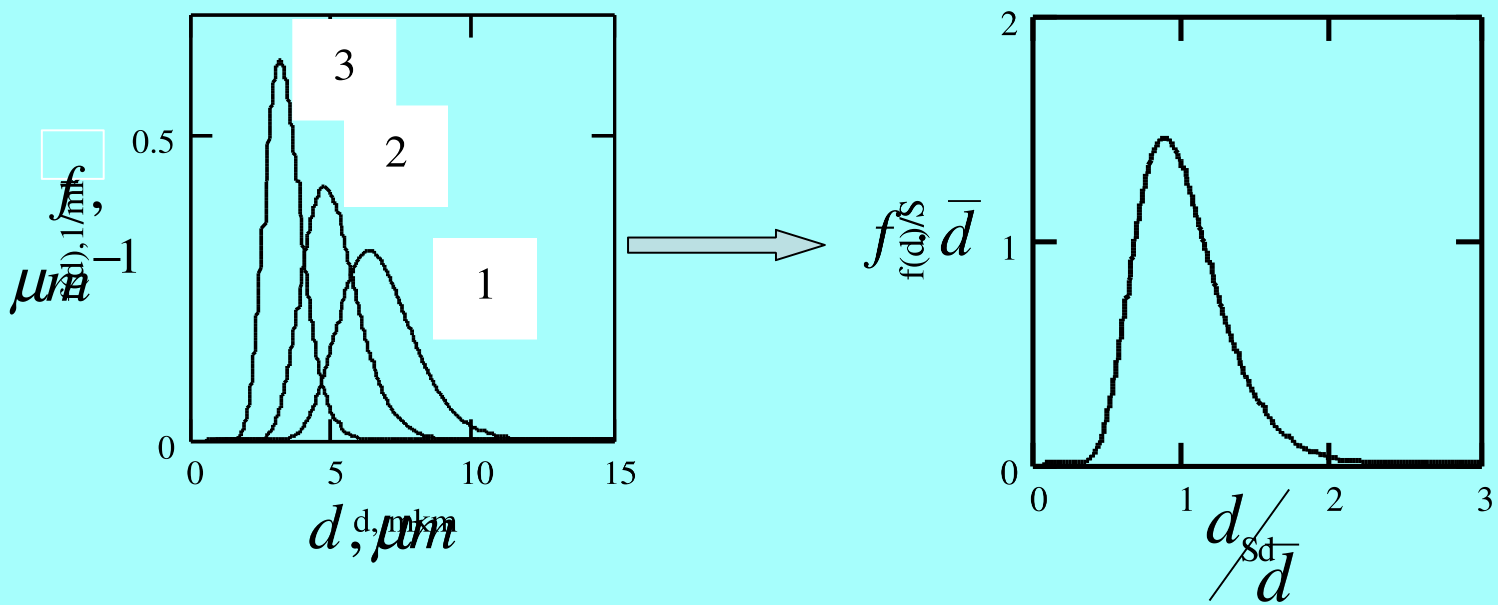
Ideal Plasticity Land

Model material does not fractures or hardens in the range of very large plastic deformations under pressure. In other words materials become ideally plastic.



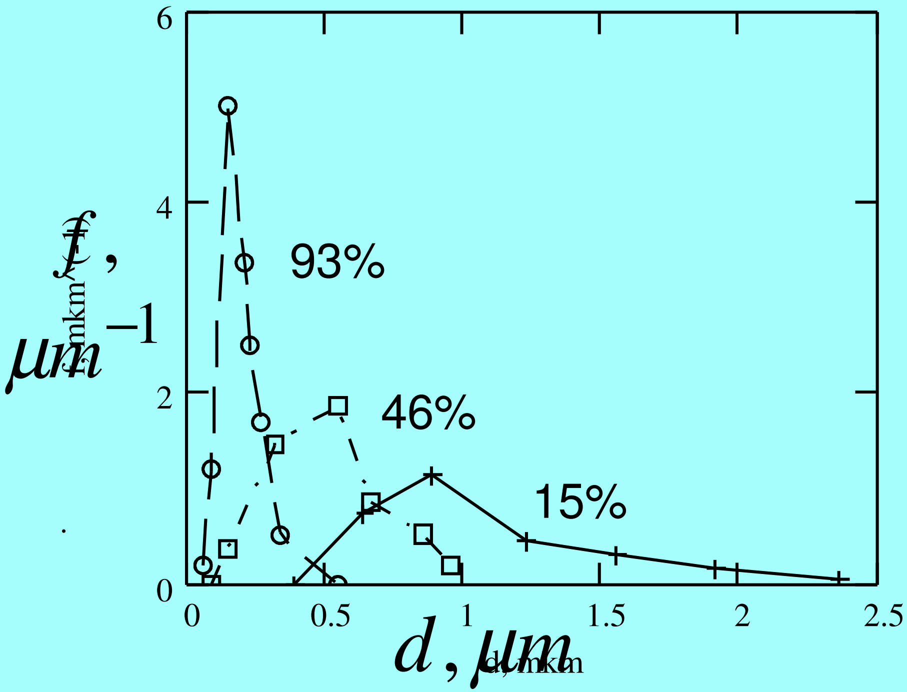
(ii)

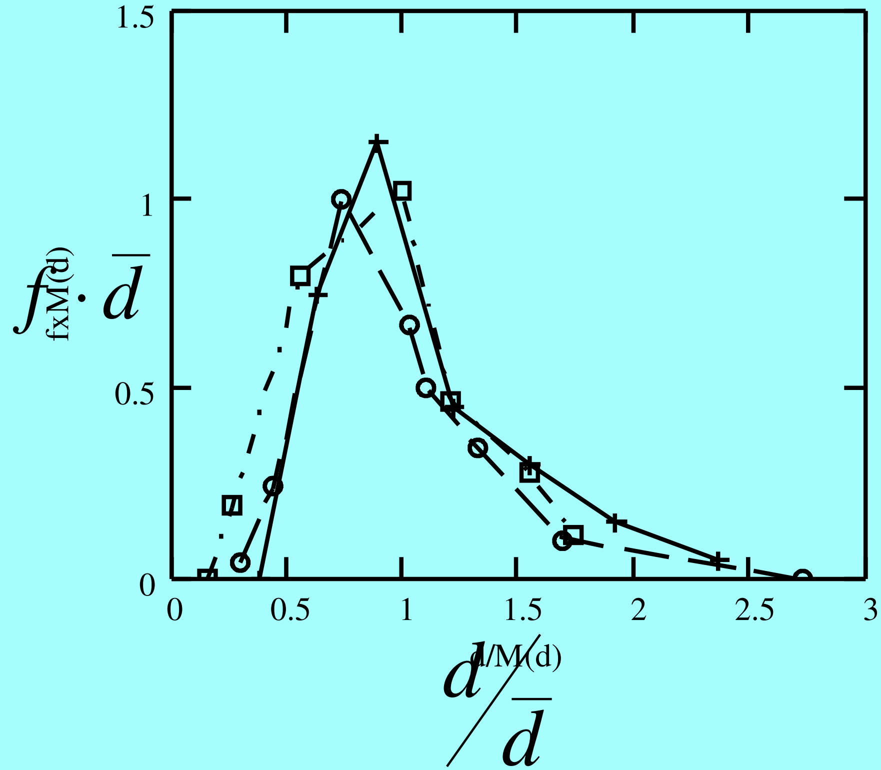
During the self-similar stage, the distribution of fragment sizes is self-similar. This implies that the distributions for different deformation stages must be the same in the normalized coordinates.

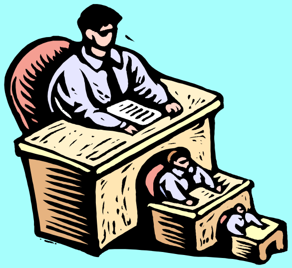


Self-similarity of Experimentally Obtained Distributions

Cu, torsion
(V.Panin et al., 1985)







(iii)

Self-similarity implies lognormal distribution for the fragments sizes (according to A. Kolmogorov, 1941)

$$f(d)=\begin{cases}\dfrac{1}{d\kappa\sqrt{2\pi}}\exp\left(-\dfrac{\left(\ln\left(\dfrac{d}{\overline{d}}\right)+0.5\kappa^2\right)^2}{2\kappa^2}\right), & if\ d>0\\[2ex] 0, if \quad d\le 0\end{cases}$$

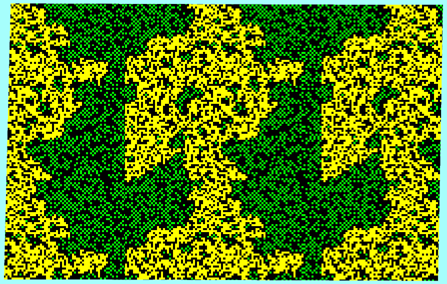
d – fragment size; $\overline{d}$ – average fragments size

κ – parameter

(iv)

During the self-similar stage of grain refinement, the fragment boundary mesh in the cross-section of the specimen represents a fractal set with dimension η, $1<\eta<2$.

Fractal set

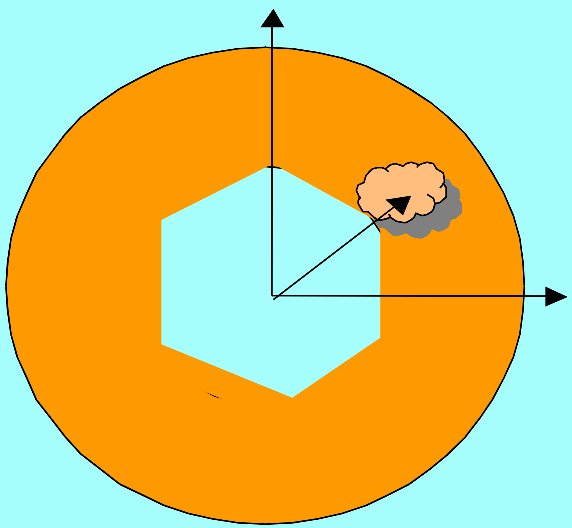


Moreover, the boundary length per unit of cross-section area and the average fragment size are related via the following equation

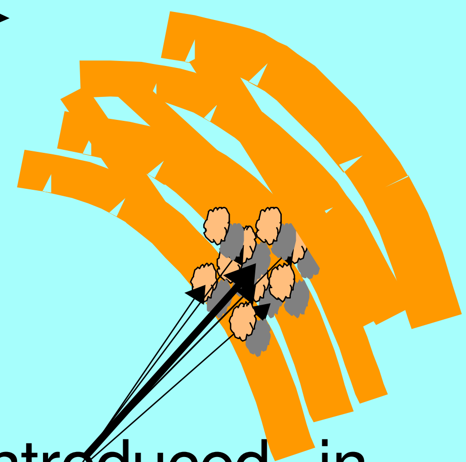
$$S \sim \frac{1}{\bar{d}^{\eta-1}}$$

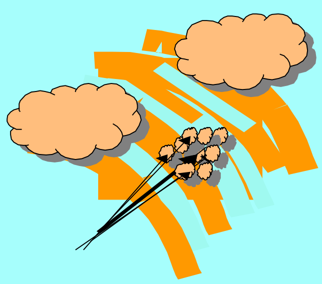
$1<\eta<2$ - fractal dimension. During the self-similar stage η is constant

Thick Yield Surfaces



A material with such structure has the Thick Yield Surface.





Such surfaces were introduced in Beygelzimer Y., et al., *Philosophical Magazine* A, **79**, N10, (1999)

(v)

When sufficiently many indivisible fragments of size d_c appear, the self-similarity of the boundary mesh gets violated. In this case

$$S \sim \frac{1}{\bar{d}}$$

(vi)

If we assume that under large plastic deformations

$$\sigma \sim S$$

then we obtain the Hall-Petch relationship for the self-similar stage of grain refinement:

$$\sigma \sim \frac{1}{\bar{d}^{\nu}}$$

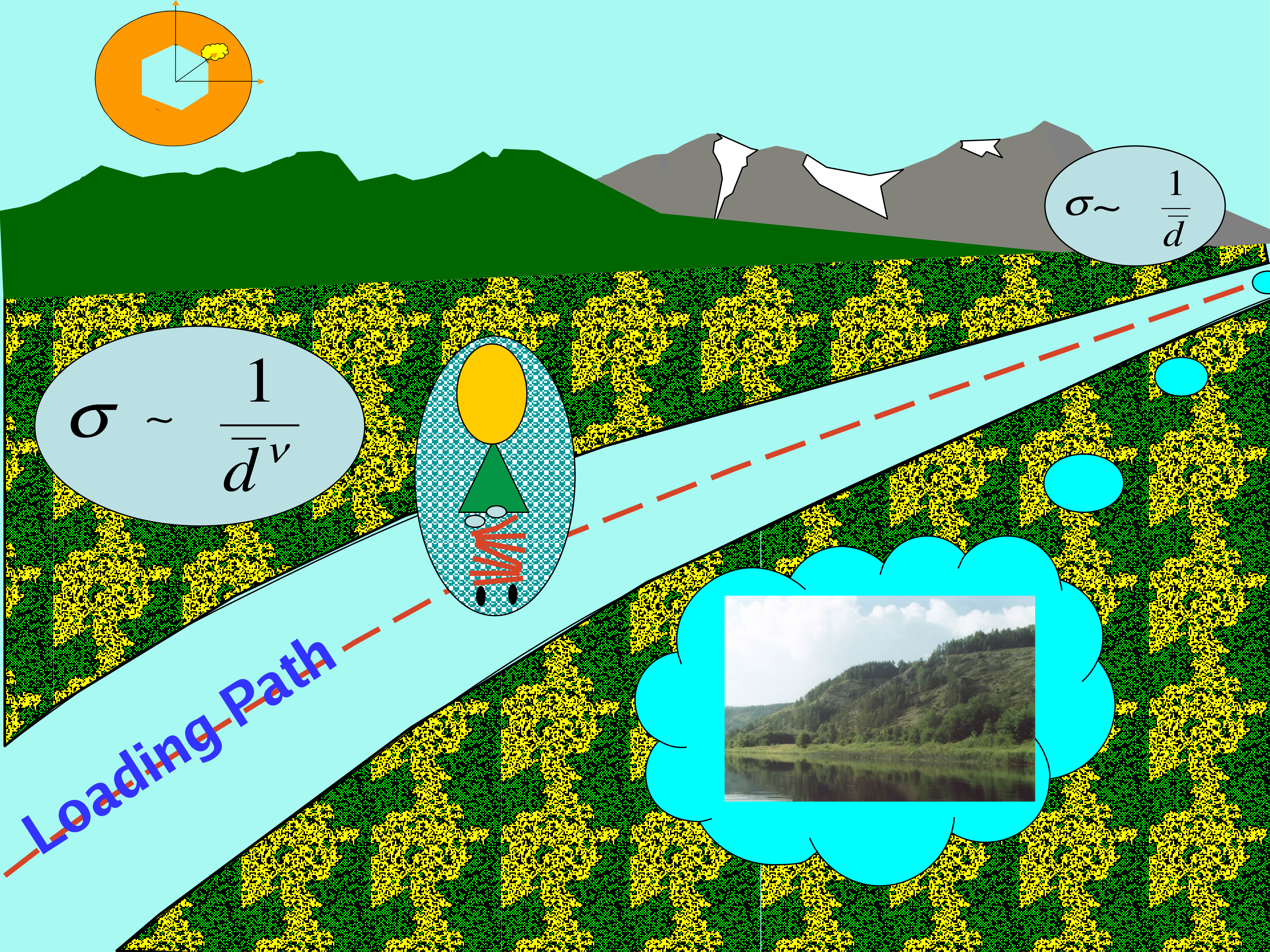
were $\nu = \eta - 1, \qquad 0 < \nu < 1$

During the self-similar stage ν is constant

(vii)

When sufficiently many indivisible fragments of size d_c appear, we have

$$\sigma \sim \frac{1}{\bar{d}}$$

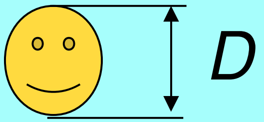


$\sigma \sim \frac{1}{\bar{d}}$
$\sigma \sim \frac{1}{\bar{d}^{\nu}}$
Loading Path

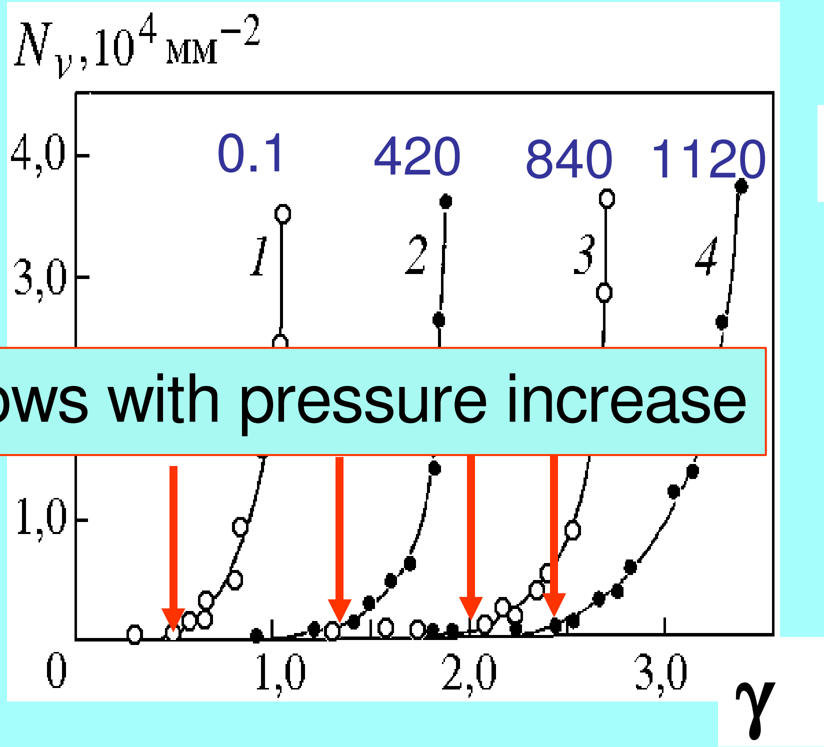
Grain refinement

At the self-similar stage $\left(d_c << d << d_0\right)$

$$S \sim \left(\frac{N_c \cdot \gamma_p(p)}{D \cdot \gamma_c(0)}\right)^{\frac{1}{3}} \sqrt{\gamma}$$



γ_p is the value of deformation marking the stage of rapid creation of voids.



p, MPa

The γ_p grows with pressure increase

$$S \sim \left(\frac{N_c \cdot \gamma_p(p)}{D \cdot \gamma_c(0)} \right)^{\frac{1}{3}} \sqrt{\gamma}$$

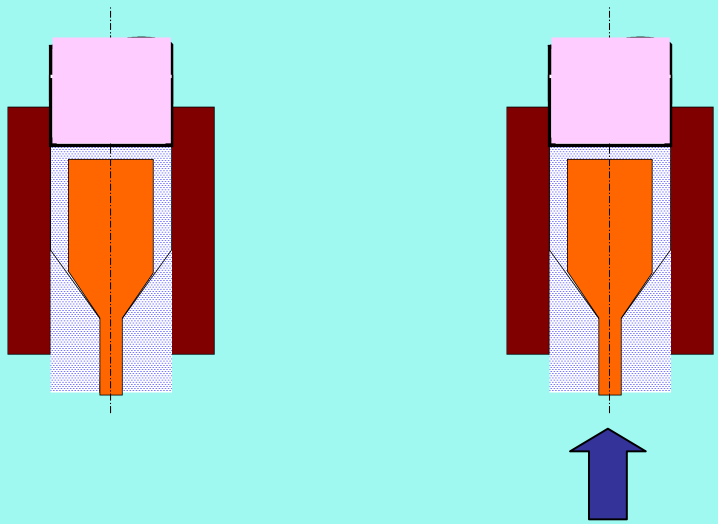
$p \Rightarrow \gamma_p \Rightarrow S$

N - number of pores per unit square of specimen cross-section; steel 1045
(experiment data Kao A.S., et al., 1990)

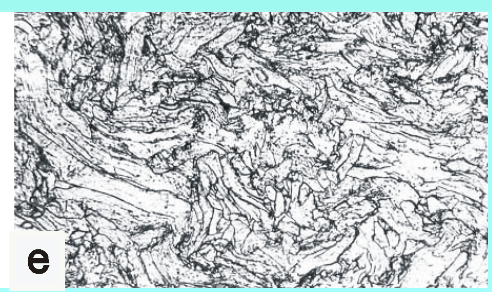
(viii)

Grain refinement intensity grows with the increase of pressure in the center of deformation.

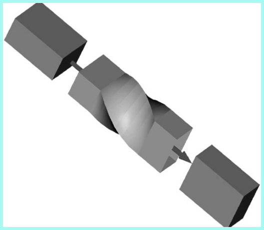
Hydroextrusion of Molybdenum (e=0.92)

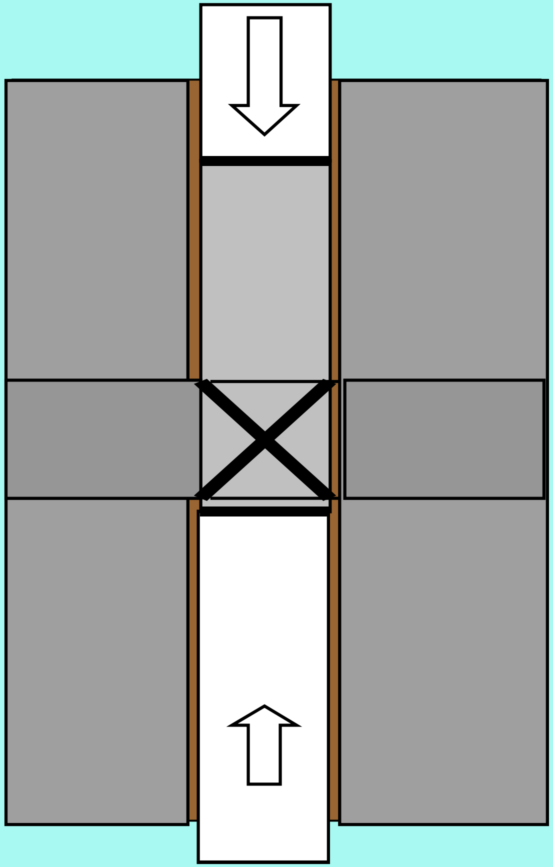


Backpressure
900 MPa



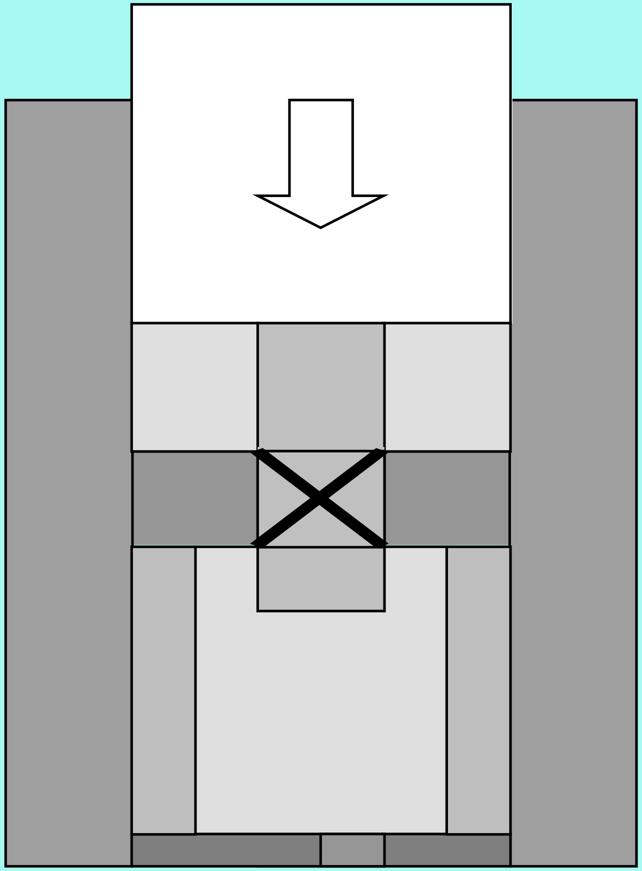
Experiment data B.Beresnev, B.Efros

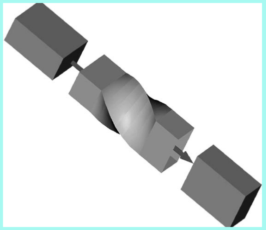


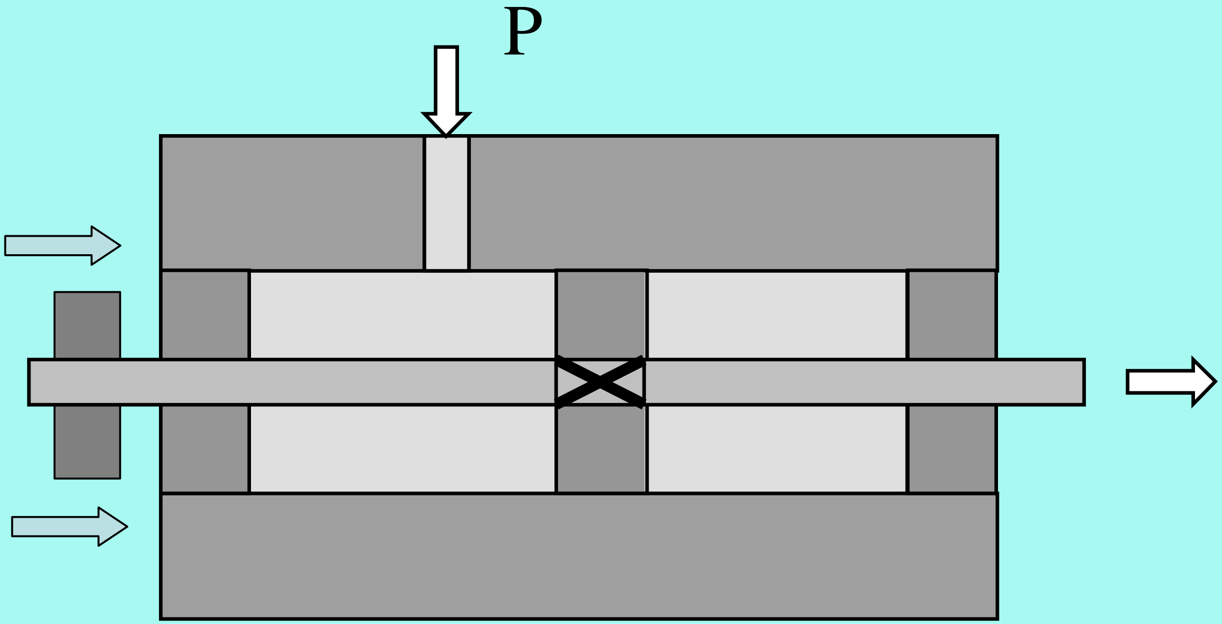


Twist Extrusion based on mechanical extrusion with backpressure

Twist Extrusion based on hydro-mechanical extrusion

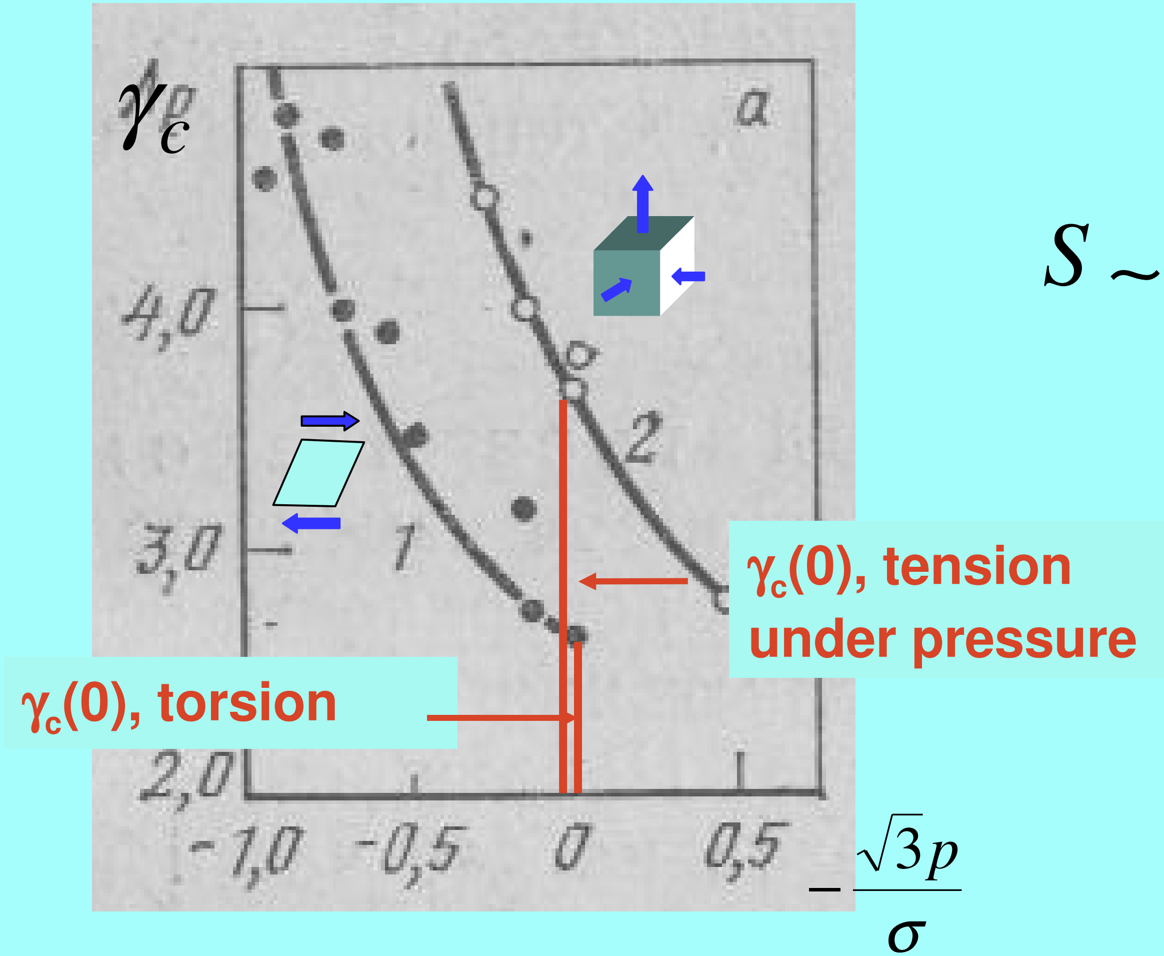






Semicontinuous hydro-mechanical Twist Extrusion

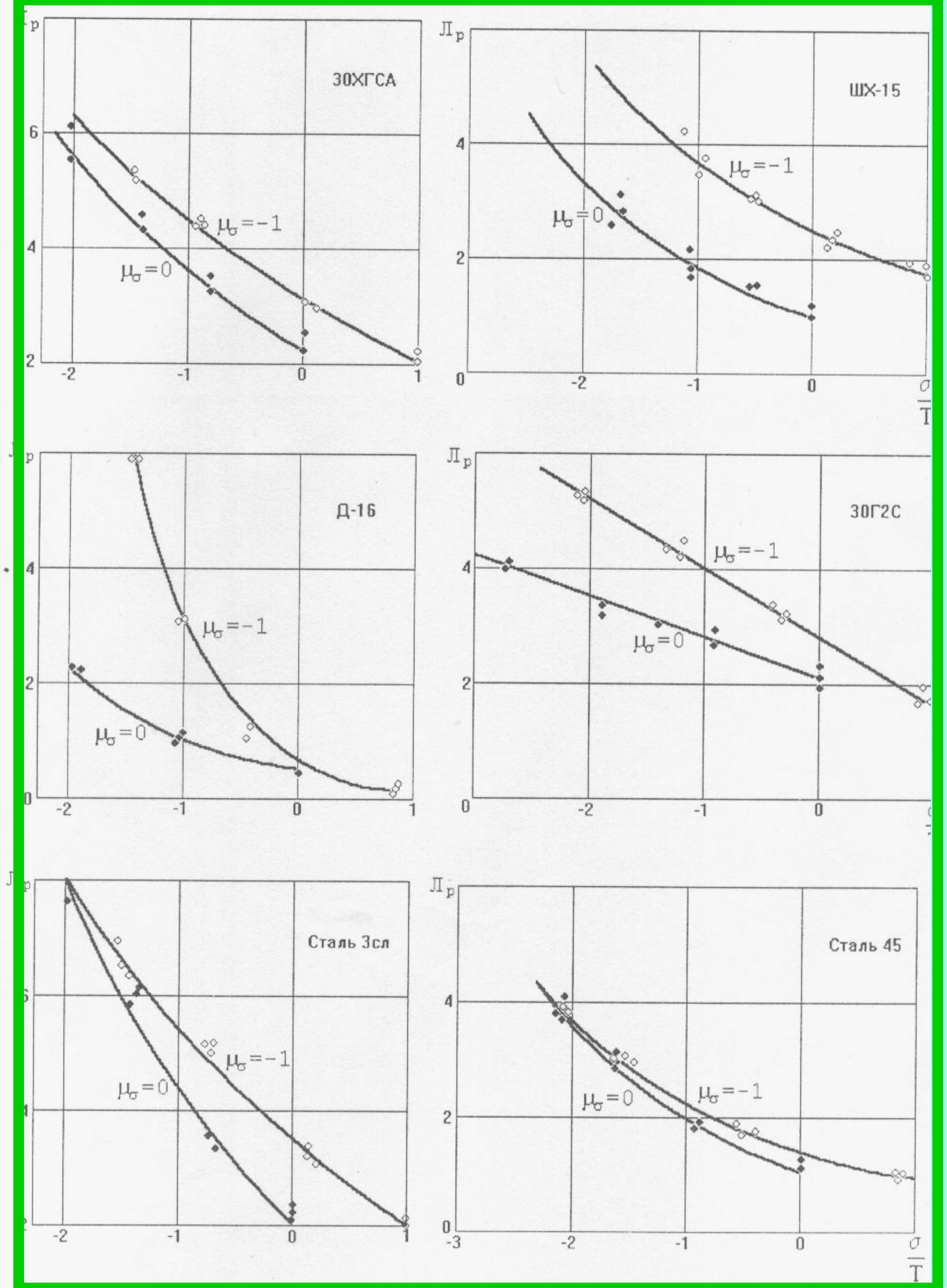
$\gamma_c(0)$ is the metal ductility at p=0



$$S \sim \left(\frac{N_c \cdot \gamma_p(p)}{D \cdot \gamma_c(0)} \right)^{\frac{1}{3}} \sqrt{\gamma}$$

$\gamma_c(0) \Rightarrow$ **S**

Ductility diagram, steel 08X18H10T
(Experiment data V.Kolmogorov, et al., 1986)

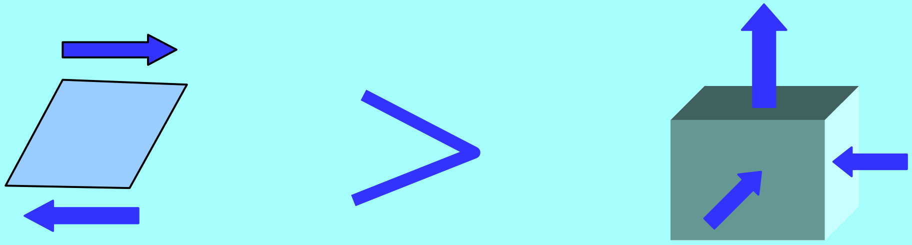


Ductility diagrams for various metals show that as a rule the $\gamma_c(0)$ for tension greater then the one for torsion.

(Experiment data V.Ogorodnikov, et al., 1999)

(ix)

Grain refinement intensity is higher for deformation schemes for which the value of $\gamma_c(0)$ is smaller. Therefore simple shear gives more intense grain refinement than uniaxial elongation.

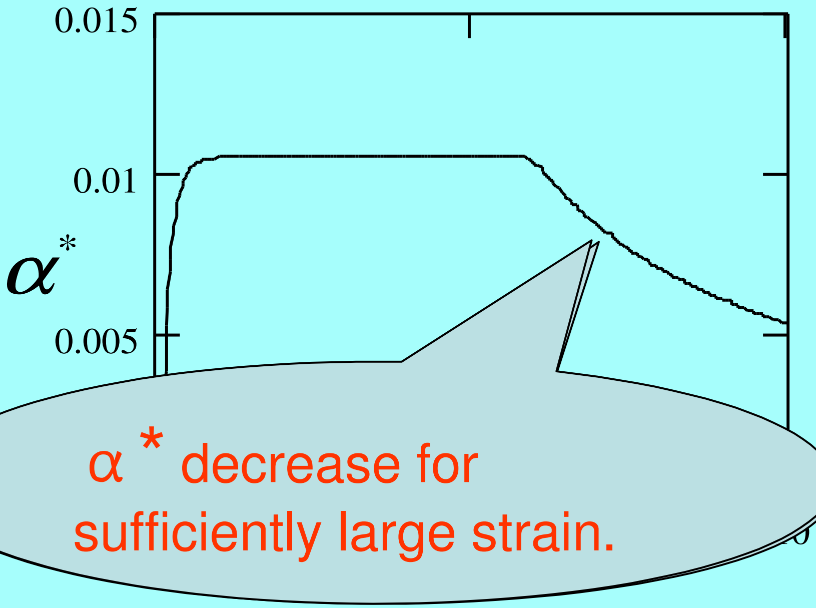


To get intense grain refinement, one needs to choose deformation schemes with small value of $\gamma_c(0)$ and perform deformation under pressure.

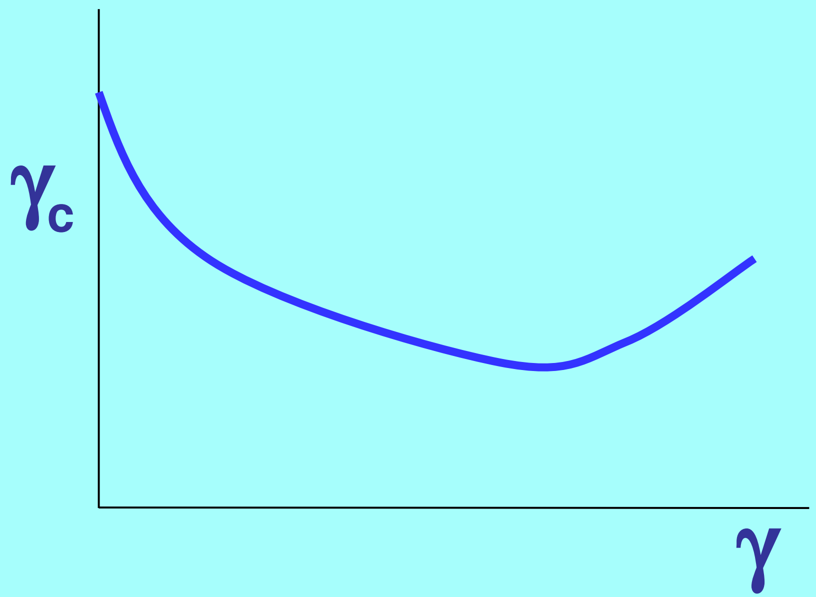
The term responsible for the birth of voids

(X)

$$\frac{d\Theta}{d\gamma} = \alpha^*(\gamma) - B\frac{p}{\sigma}\Theta \qquad \alpha^*(\gamma) = C_3\overline{N}^{\frac{3}{2}}(\gamma)\,d_c^{-3}v$$

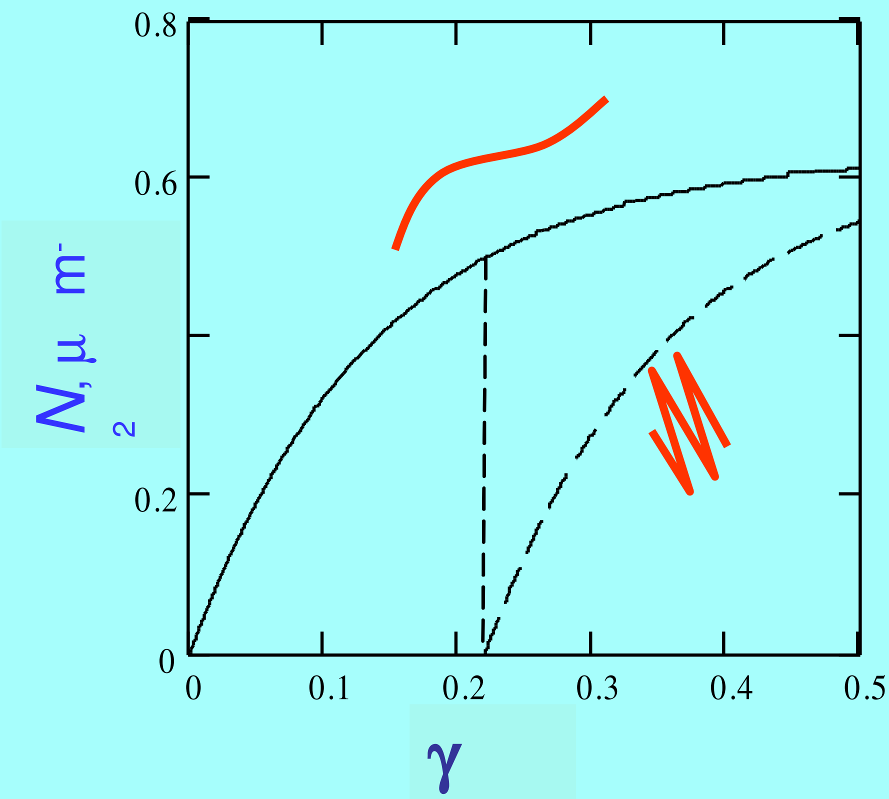


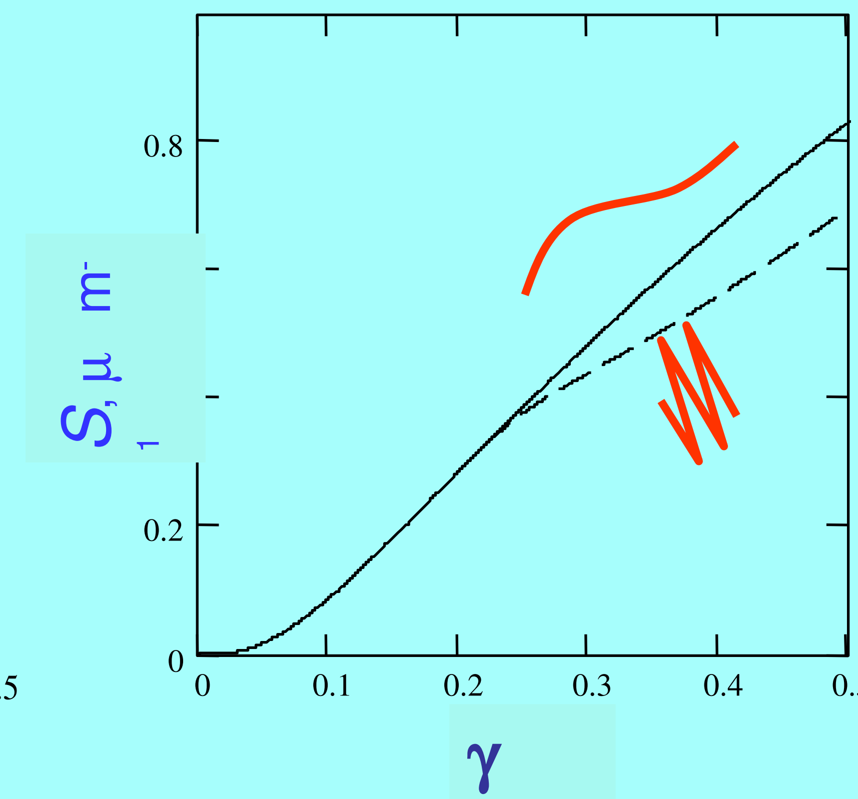
α * decrease for sufficiently large strain.



(xi)

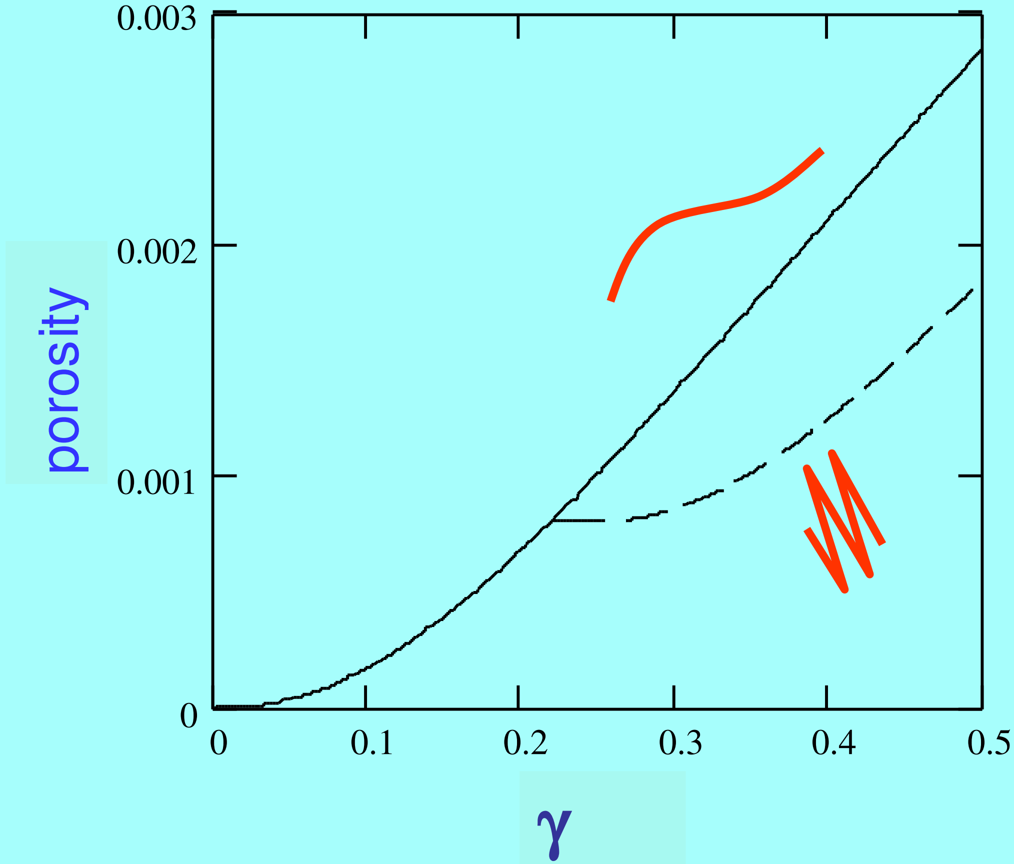
Quasi-monotone deformations provide higher grain refinement intensity than cyclic deformation.





(xii)

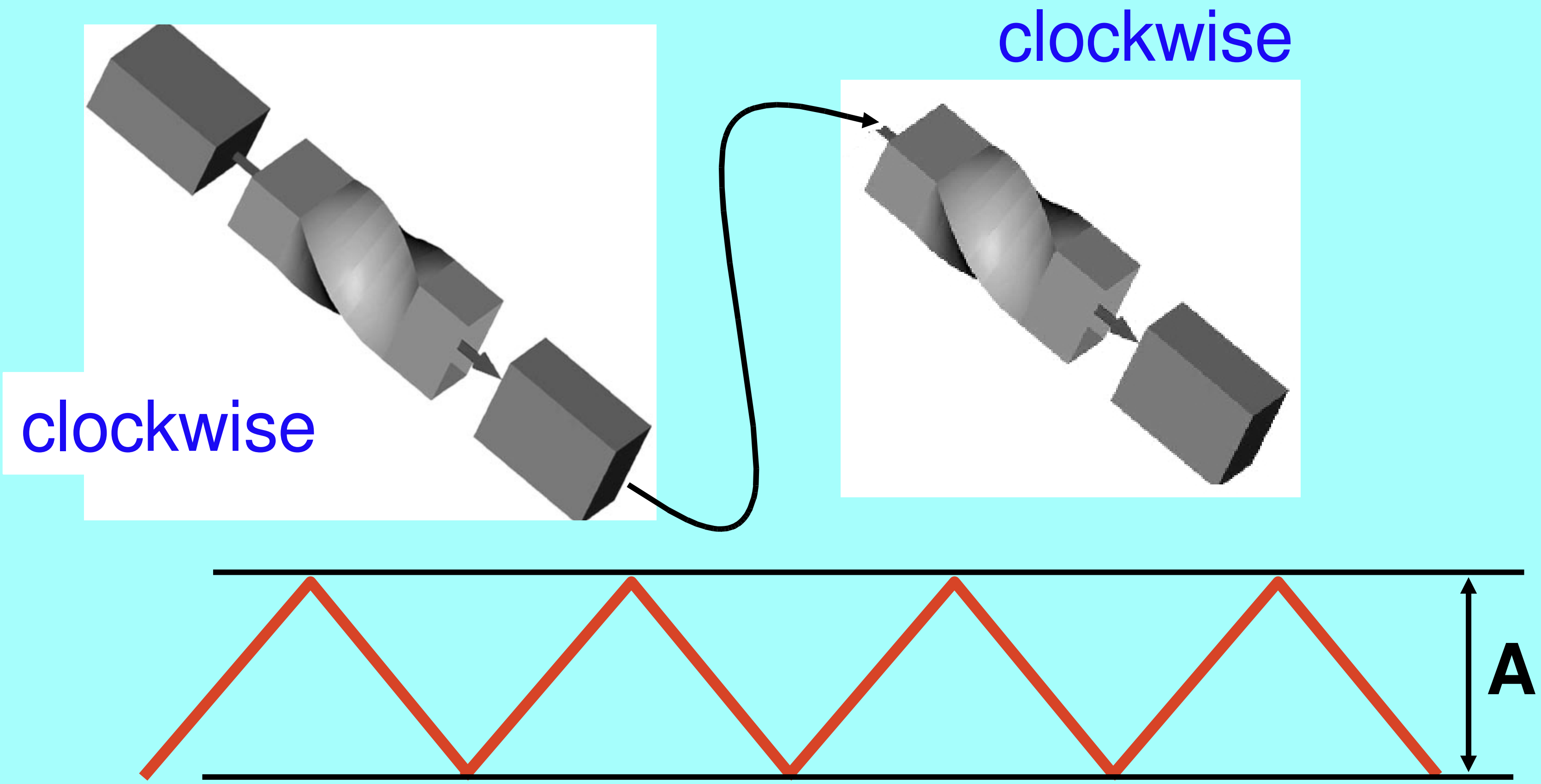
Cyclic deformations provide higher ductility than quasi-monotone deformation

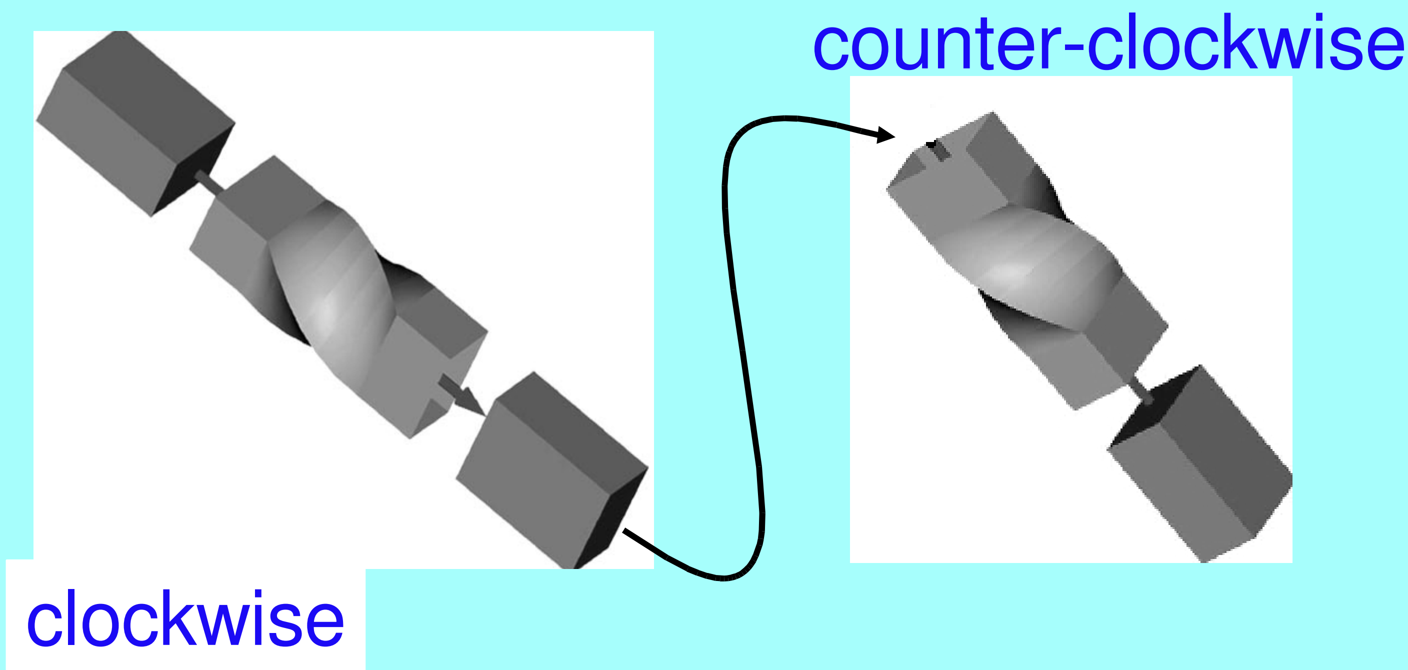


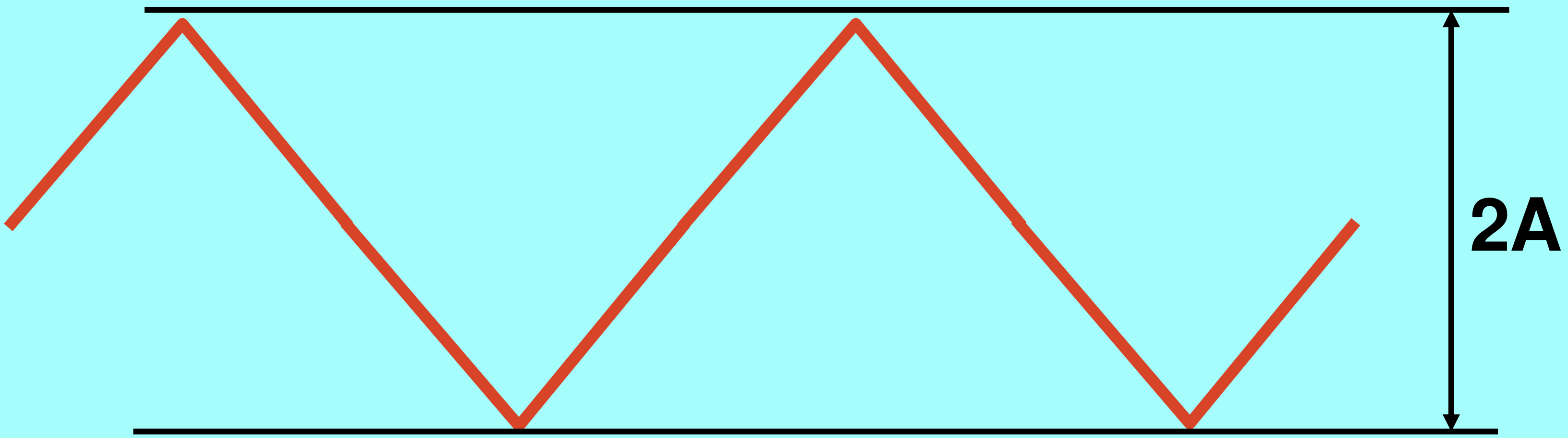
(xiii)

In order to increase the intensity of grain refinement under cyclic deformation, one has to increase the amplitude of deformation.

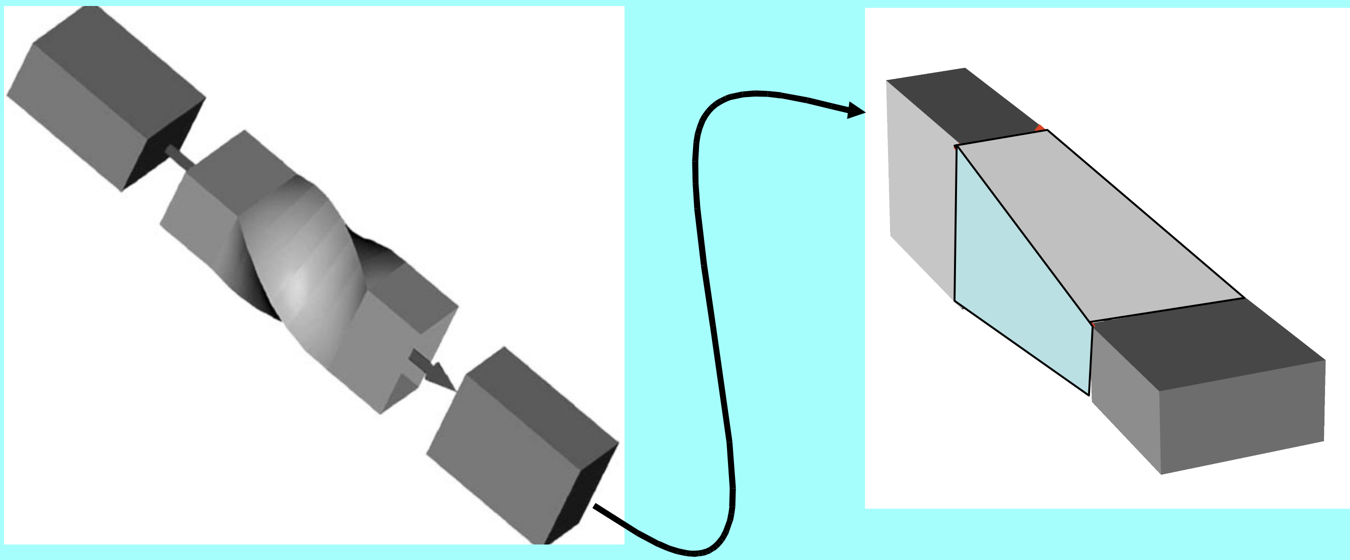
For example, in the Twist Extrusion we combine clockwise and counter-clockwise dies.


clockwise
clockwise
A


counter-clockwise
clockwise


2A

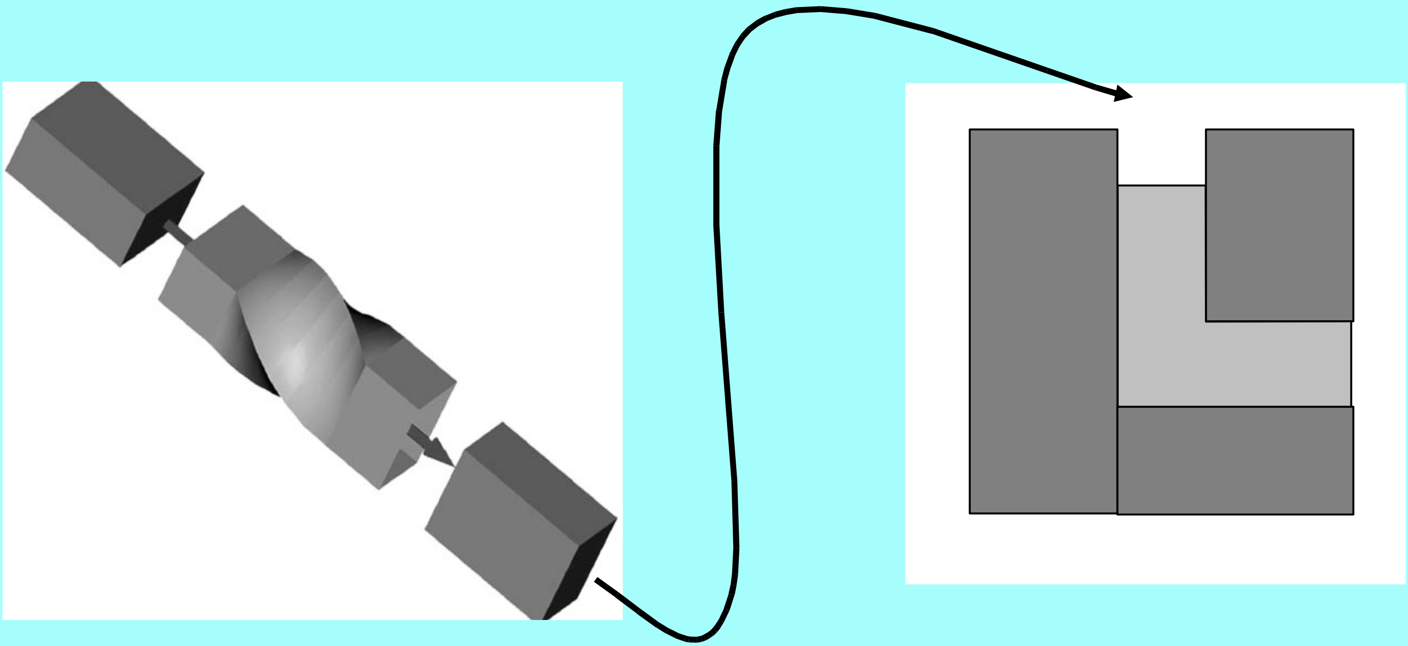
To avoid cyclic deformation we combine the Twist Extrusion with the Spread Extrusion



Twist Extrusion

Spread Extrusion

We think, that the good results will be given by the combination of Twist Extrusion with Equal Channel Angular Extrusion

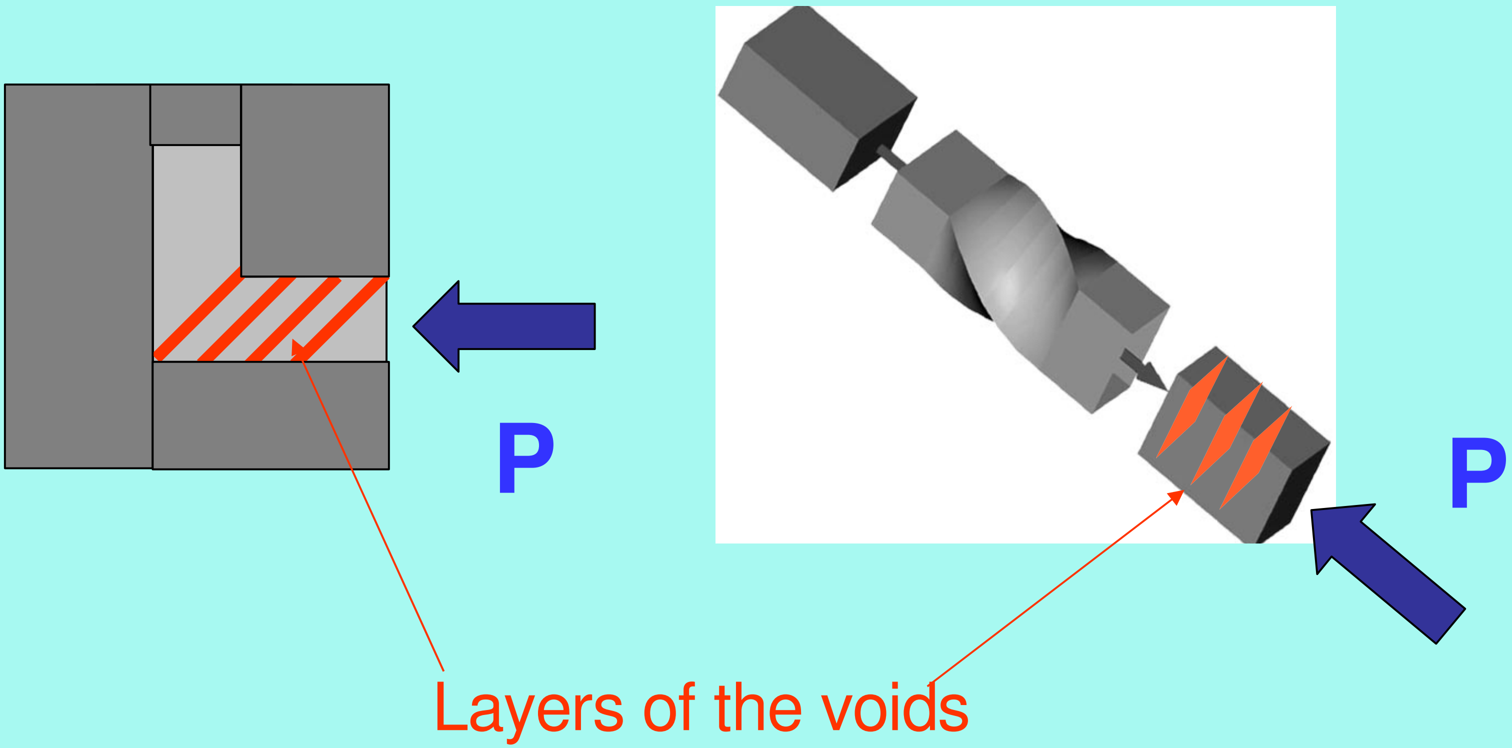


(xiv) **Strain localization**

Strain localization is a manifestation of the interdependency between macro- and micro- levels.

One of the possible causes of strain localization during simple shear is an avalanche-like increase in porosity corresponding to a small metal strengthening. This is accompanied by the appearance of a voids layer along the shift plane. This decreases metal ductility in the direction perpendicular to this plane, and in certain cases can fracture the specimen along the plane.

The analysis of the model shows that a sufficiently high pressure in the center of deformation prevents this undesirable effect.

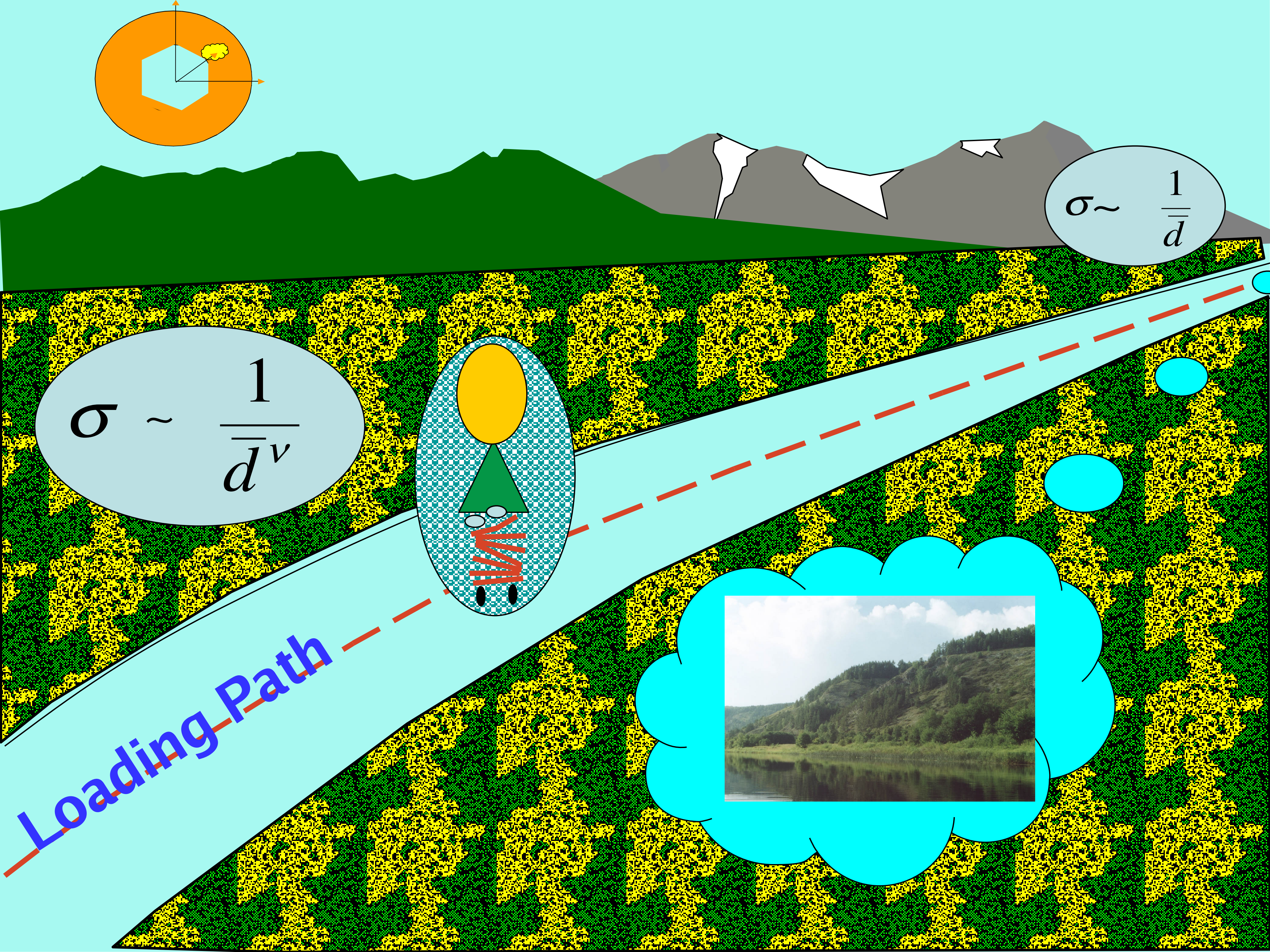

P
P
Layers of the voids

Main consequences

- Sufficiently large pressure allows one to prevents strain localization related with formation of the layers of the voids.
- The intensity of grain refinement increases with the increase of pressure in the center of deformation
- To achieve intense grain refinement, one needs to choose deformation scheme with a small value of $\boldsymbol{\gamma_c(0)}$ and perform deformation under pressure.
- The exponent ν in the Hall-Petch law is related to the fractal dimension of the high-angle boundary mesh by the relation $\nu = \eta - 1$

Main consequences

- Quasi-monotone deformations provide higher grain refinement intensity than cyclic deformations
- In order to increase the intensity of grain refinement under cyclic deformation, one has to increase the amplitude of deformation.
- Cyclic deformations provide higher ductility than quasi-monotone deformations



$\sigma \sim \frac{1}{\bar{d}}$
$\sigma \sim \frac{1}{\bar{d}^{\nu}}$
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