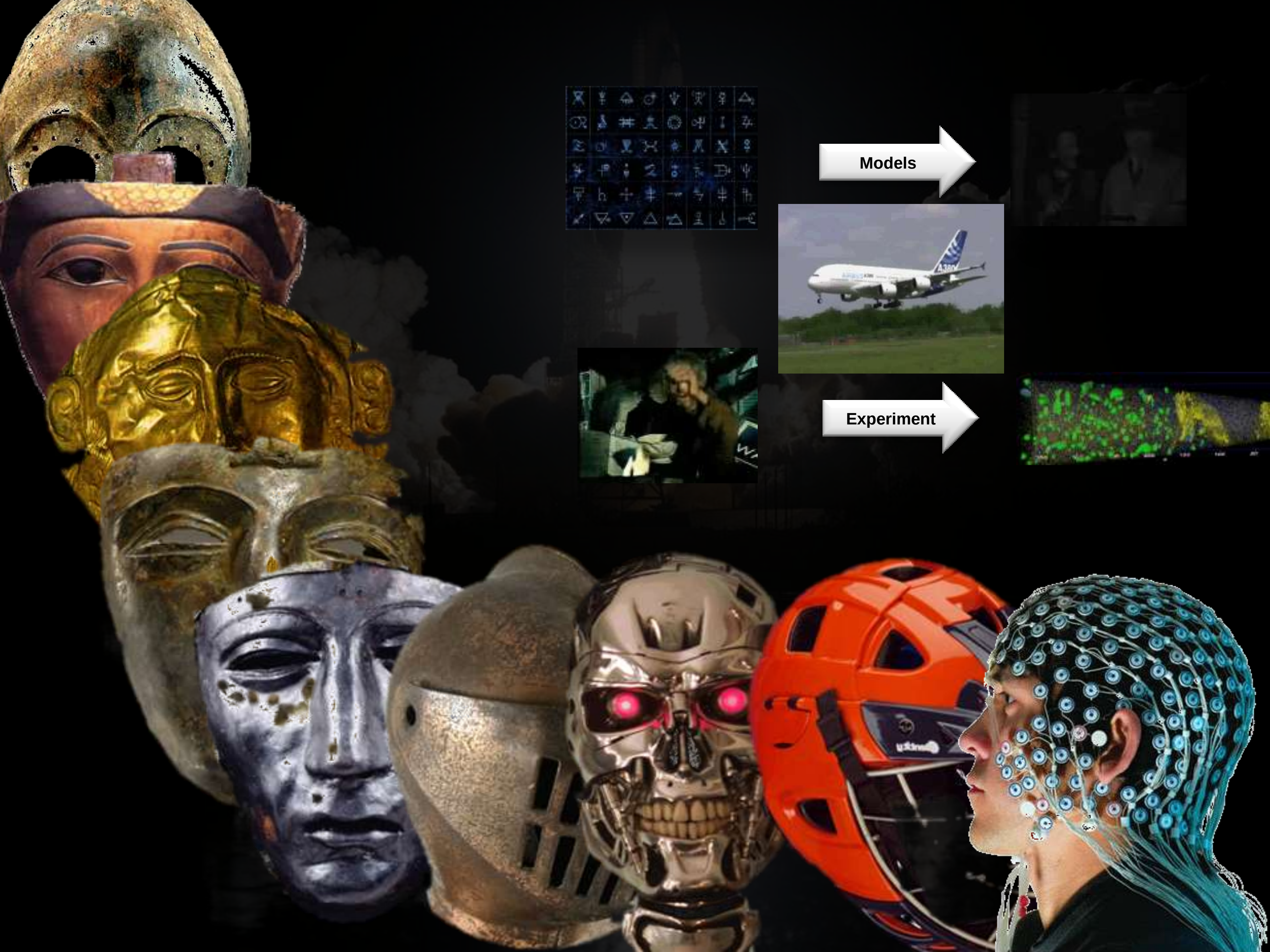
Modeling of Materials: Development with Simulation – Discoveries through Simulation

F. Roters, T. Hickel, J. Neugebauer, M. Friak, C. Tasan, M. Diehl, D. Raabe

Max-Planck-Institut
für Eisenforschung GmbH
Düsseldorf, Germany

MAX-PLANCK-GESELLSCHAFT

Dierk Raabe, DFG Winterschool, 14. Feb. 2017, Aachen, Germany


Models
Experiment

Answering societies' grand challenges with complex alloys

70% of all **Industrial Innovations** are associated with progress in **Materials Science**

Key fields: energy, transportation, information, health, safety, infrastructure

3.5 billion € turnover per day in the EU
World Trade Organisation

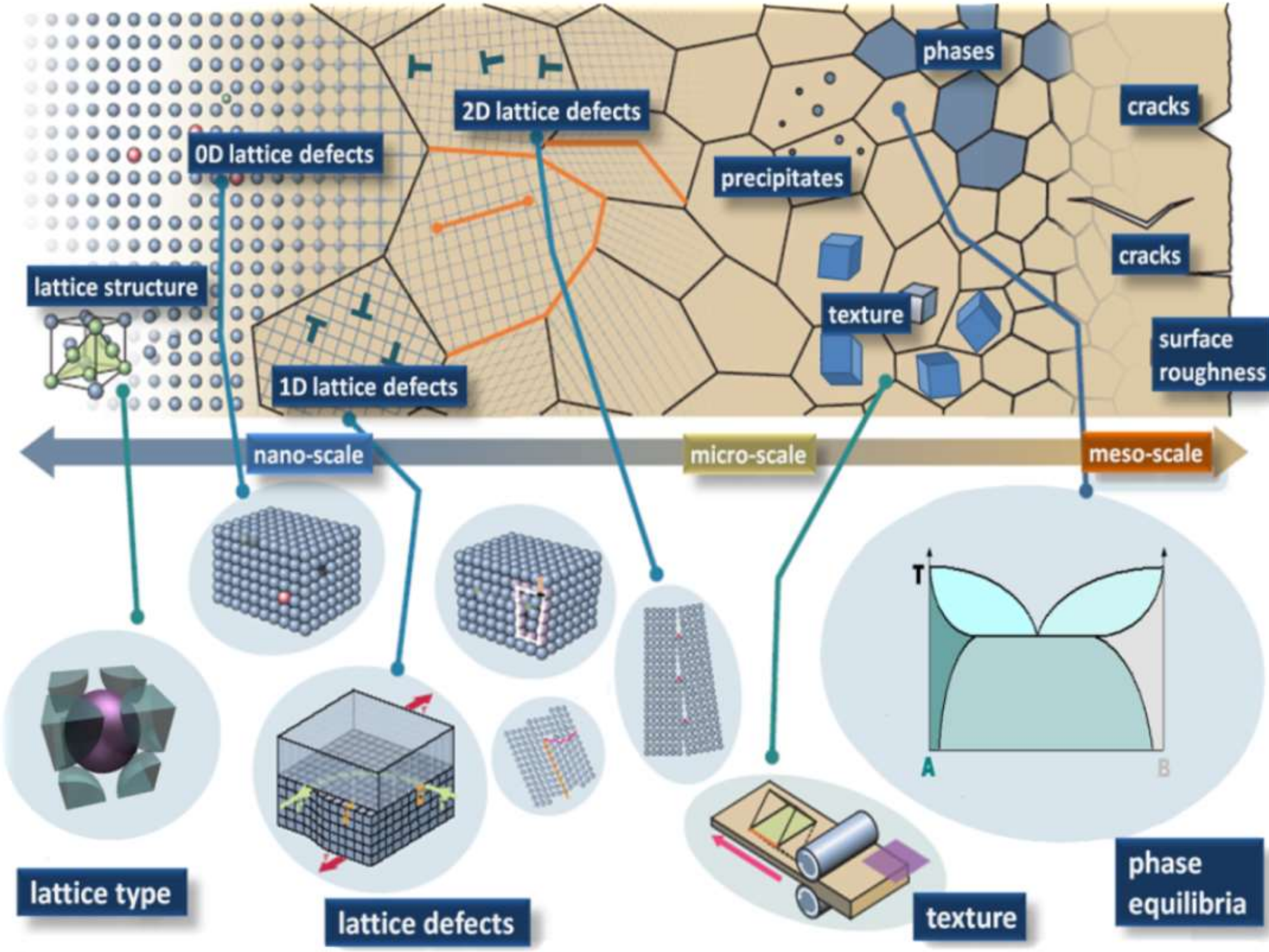
10^{70} unknown alloys (we use only 1000 alloys)

Mission:

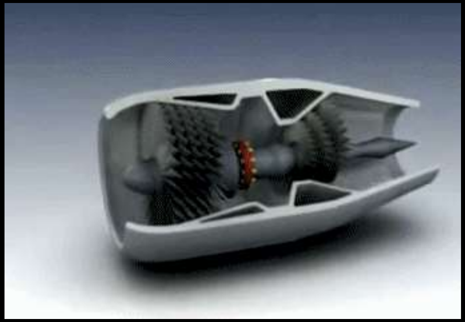
Understand and design <u>complex</u> nanostructured <u>materials</u> under real <u>environments</u> down to <u>atomic</u> scale by utilizing <u>modeling and simulation</u>

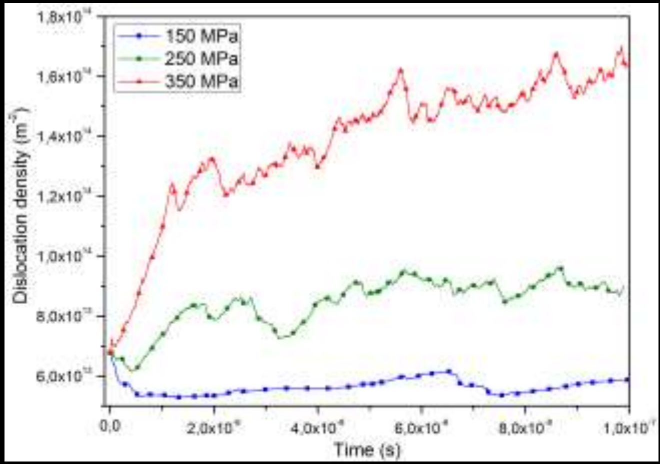
Courtesy Airbus, GE, Siemens, Ford, TKS, EADS, Titanium

Scientific mission: complex materials in real environments



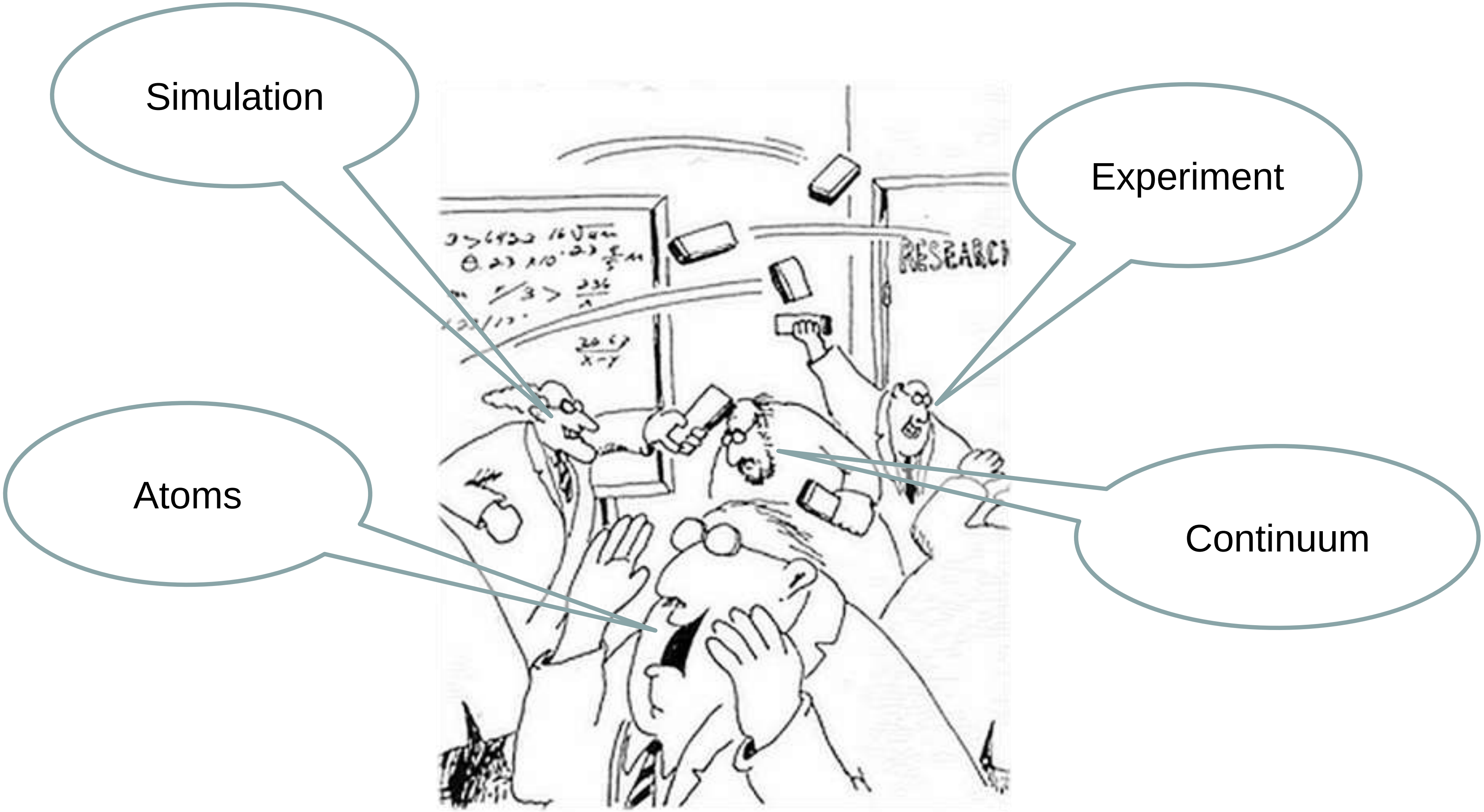
Example: 4th generation superalloys for turbine blades (SFB / TR 103)





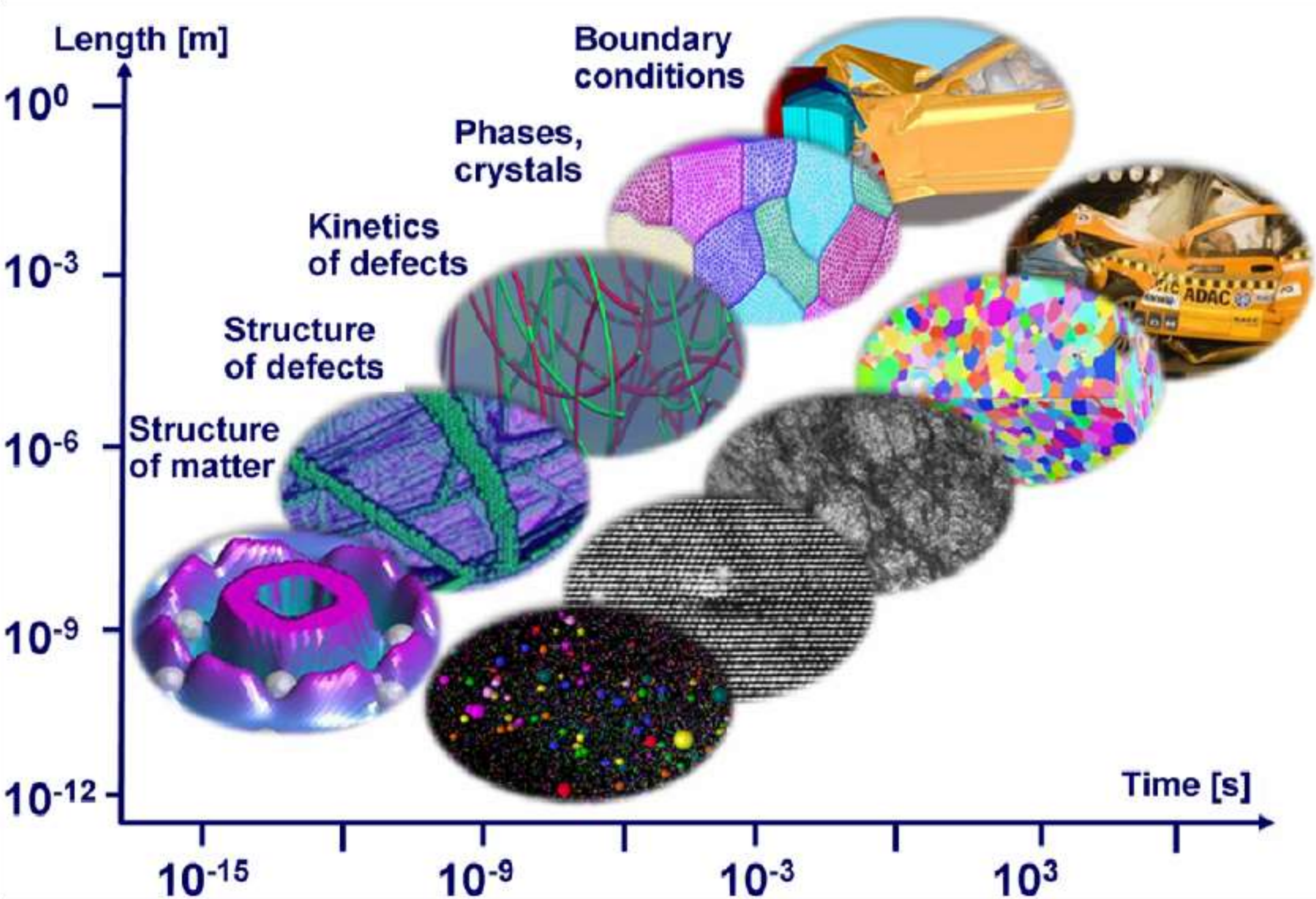
sources GE; FAU Erlangen Nürnberg und RU Bochum

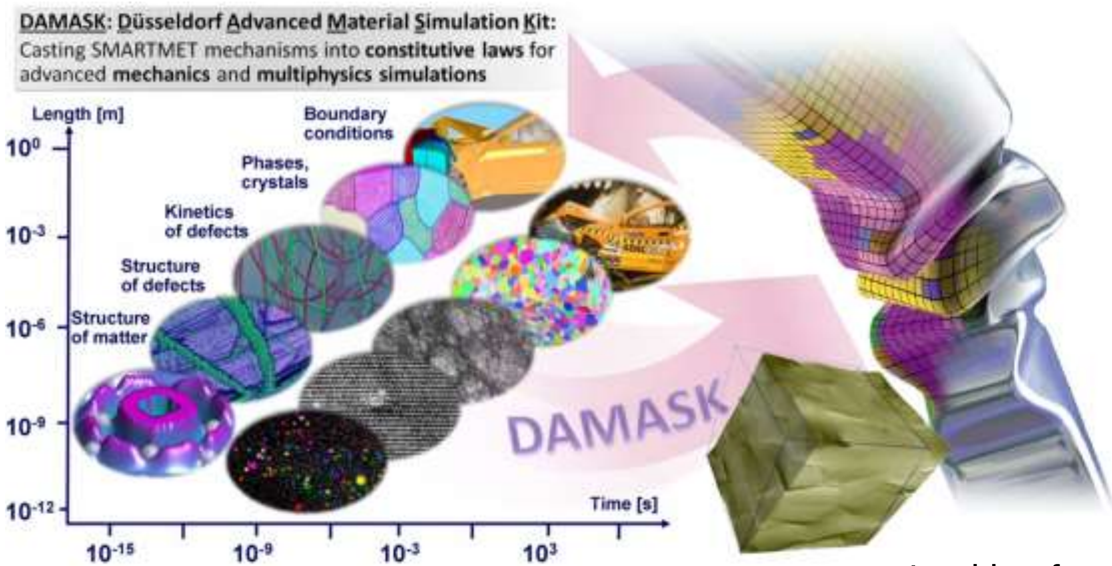
ICME: Integrated Computational Materials Engineering



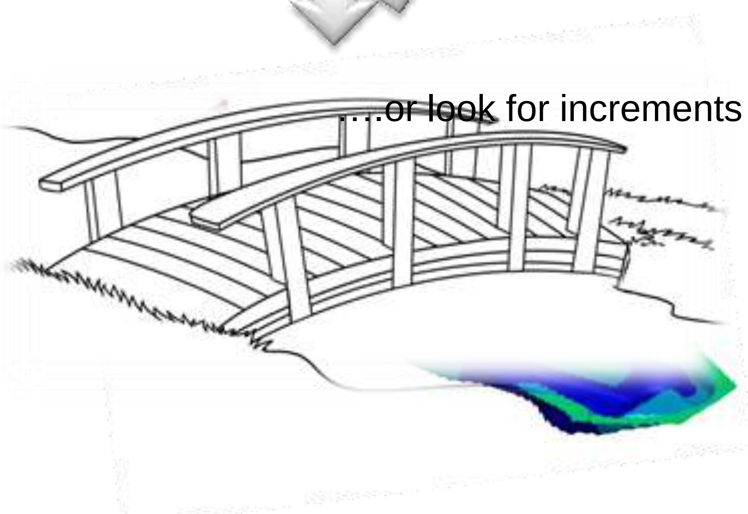
G. Larson

Multiscale Modeling and Experimentation

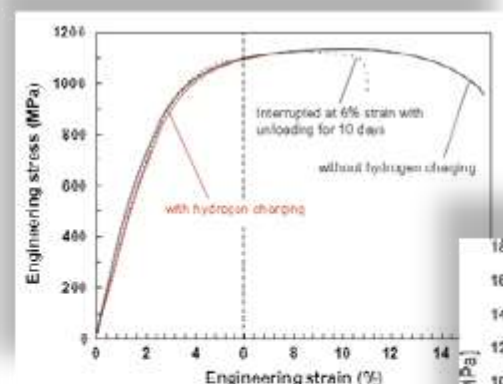




Looking for multi-mechanisms / alloy trends ….

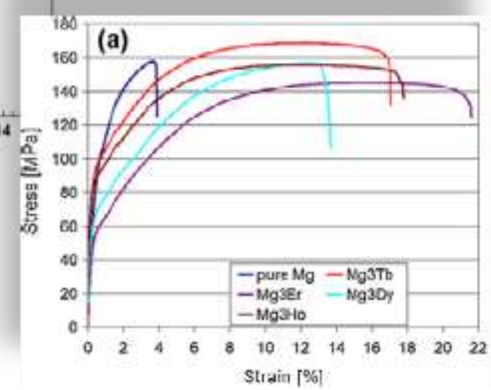


….or look for increments ?



HELP
HEV
HEDE
HYDRID

Pyramidal slip
Corrosion



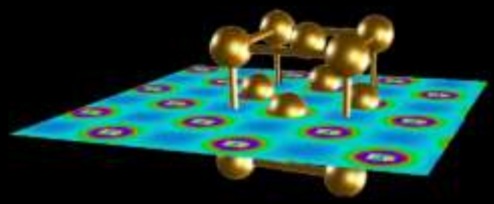
Overview

- Some basic methods
  - Atomistic
  - Monte Carlo
  - Dislocations
  - Polycrystal mechanics

- Ab-initio informed constitutive models
  - Elasticity: from DFT to Homogenization
  - Atomistically informed simulation: from APT to MD
  - From DFT to dislocation rate models and yield surfaces

DFT: Density Functional Theory; APT: Atom Probe Tomography; MD: Molecular Dynamics; RVE: Representative Volume Element; ICME: Integrated Computational Materials Engineering

- MOST EXACT KNOWN MATERIALS THEORY
- COMBINE TO ATOMIC SCALE EXPERIMENTS
- OBTAIN DATA NOT ACCESSIBLE OTHERWISE
- CAN BE USED AT CONTINUUM SCALE
- ELECTRONIC RULES FOR ALLOY DESIGN: ADD ELECTRONS RATHER THAN ATOMS



Counts, Friák, Raabe, Neugebauer: Acta Mater. 57 (2009) 69 h/(2π)

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r)+U(r)\psi(r)=E\,\psi(r)$$

square $|\psi(\underline{r})|^2$ of the wave function $\psi(\underline{r})$ at position $\underline{r} = (x,y,z)$
is a measure of the probability (Aufenthaltswahrscheinlichkeit)

many particles

$$\left(-\frac{\hbar^2}{2}\sum_i\frac{1}{m_i}\nabla_i^2+U(r_i)\right)\psi(r_i)=E\,\psi(r_i)$$

time-independent Schrödinger equation for many particles

i Electrons: Mass m_e ; Charge $q_e = -e$; Coordinates r_{ei}
j Cores: Mass m_n ; Charge $q_n = ze$; Coordinates r_{nj}

$$\left(-\frac{\hbar}{2m_e}\sum_i \nabla_i^2 - \frac{\hbar}{2m_n}\sum_j \nabla_j^2 + \sum_{\substack{i1,i2\\ i1\neq i2}} \frac{e^2}{4\pi\varepsilon_0 \left| r_{e_{i1}} - r_{e_{i2}} \right|} + \sum_{\substack{j1,j2\\ j1\neq j2}} \frac{z_{j1} z_{j2} e^2}{4\pi\varepsilon_0 \left| r_{n_{j1}} - r_{n_{j2}} \right|} + \sum_{i,j} \frac{z_j e^2}{4\pi\varepsilon_0 \left| r_{e_i} - r_{n_j} \right|} \right) \psi\left(r_{e_i}, r_{n_j}\right) = E\,\psi\left(r_{e_i}, r_{n_j}\right)$$

Adiabatic Born-Oppenheimer approximation

Decoupling of cores and electrons

$$\psi(\mathrm{r_e},\mathrm{r_n}) = \varphi(\mathrm{r_e})\phi(\mathrm{r_n})$$

Electrons

$$\left(-\frac{\hbar}{2m_e}\sum_i \nabla_i^2 + \sum_{\substack{i1,i2\\ i1\neq i2}} \frac{e^2}{4\pi\varepsilon_0 \left| r_{e_{i1}} - r_{e_{i2}} \right|} + \sum_{i,j} \frac{z_j e^2}{4\pi\varepsilon_0 \left| r_{e_i} - r_{n_j} \right|} \right) \varphi(r_{e_i}) = E\varphi(r_{e_i})$$

Atom cores

$$\left(-\frac{\hbar}{2m_n}\sum_j \nabla_j^2 + \sum_{\substack{j1,j2\\ j1\neq j2}} \frac{z_{j1} z_{j2} e^2}{4\pi\varepsilon_0 \left| r_{n_{j1}} - r_{n_{j2}} \right|} + \sum_{i,j} \frac{z_j e^2}{4\pi\varepsilon_0 \left| r_{e_i} - r_{n_j} \right|} \right) \phi(r_{n_j}) = E\phi(r_{n_j})$$

Adiabatic Born-Oppenheimer approximation: classical mechanics

- Instead of using Quantum mechanics, we can use classical Newtonian mechanics to model our system.
- This is a simplification of what is actually going on, and is therefore less accurate.
- To alleviate this problem, we use numbers derived from QM for the constants in our classical equations.

For each atom in every molecule, we need:

- Position (r)
- Momentum ($m + v$)
- Charge (q)
- Bond information (which atoms, bond angles, etc.)

From potential to motion

To run the simulation, we need the force on each particle.

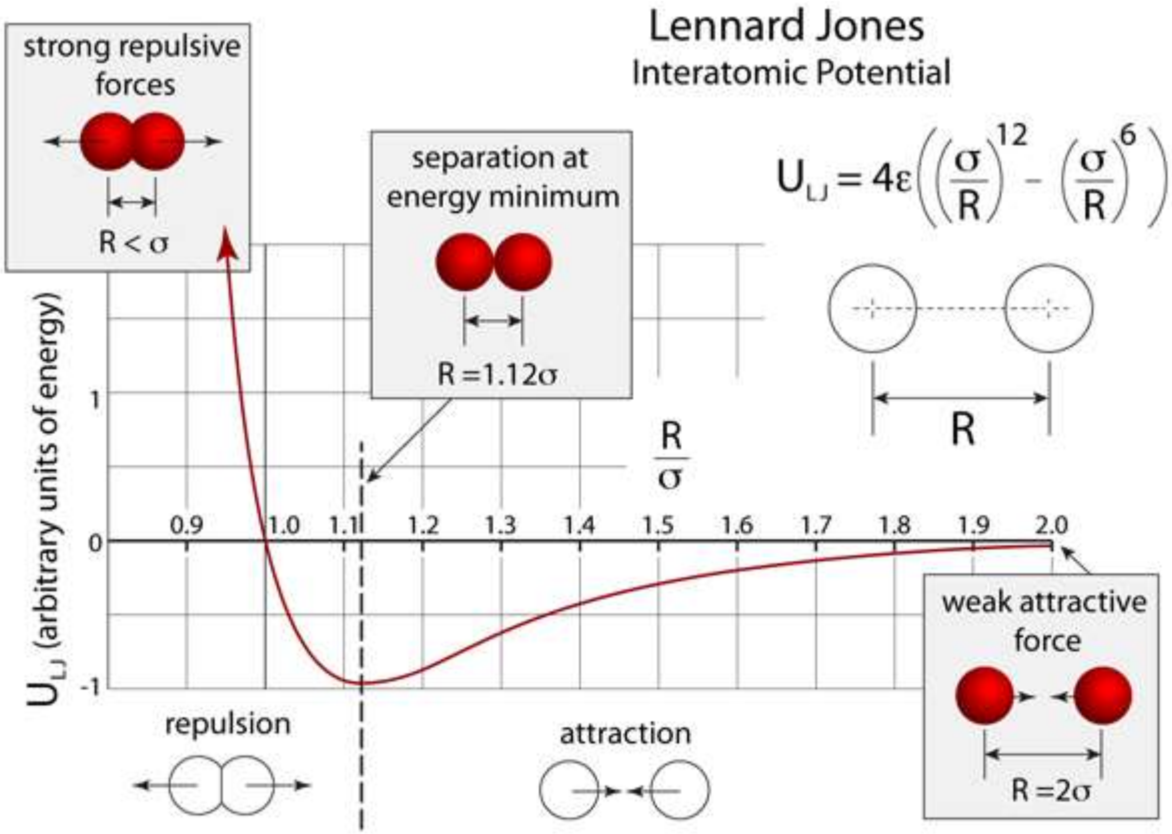
$$F_i = m_i a_i$$

We use the gradient of the potential energy function.

$$F_i = -\nabla_i V$$

Now we can find the acceleration.

$$-\frac{dV}{dr_i} = m_i \frac{d^2 r_i}{dt^2}$$



$$F_i = -\nabla_i V$$

$$-\frac{dV}{dr_i} = m_i \frac{d^2 r_i}{dt^2}$$

Integration of equation of motion (Verlet)

The Verlet technique allows one to calculate the actual position $\boldsymbol{r}_i$ and velocity $\dot{\boldsymbol{r}}_i$ of the ith atom at time t in Cartesian coordinates (in the general Lagrange formalism the Cartesian coordinates $\boldsymbol{r}$ must be distinguished from the generalized coordinates $\boldsymbol{x}$). The displacement in the vicinity of t can be described by a Taylor expansion:

$$\boldsymbol{r}_i(t+\delta t) = \boldsymbol{r}_i(t) + \dot{\boldsymbol{r}}_i(t)\delta t + \frac{1}{2}\ddot{\boldsymbol{r}}_i(t)(\delta t)^2 + \frac{1}{3!}\dddot{\boldsymbol{r}}_i(t)(\delta t)^3 + \frac{1}{4!}\ddddot{\boldsymbol{r}}_i(t)(\delta t)^4 + \ldots$$

$$\boldsymbol{r}_i(t-\delta t) = \boldsymbol{r}_i(t) - \dot{\boldsymbol{r}}_i(t)\delta t + \frac{1}{2}\ddot{\boldsymbol{r}}_i(t)(\delta t)^2 - \frac{1}{3!}\dddot{\boldsymbol{r}}_i(t)(\delta t)^3 + \frac{1}{4!}\ddddot{\boldsymbol{r}}_i(t)(\delta t)^4 \mp \ldots$$

By adding equations (4.47) and (4.48) one obtains an expression for the position of the ith atom as a function of its acceleration,

$$\begin{aligned} \boldsymbol{r}_i(t+\delta t) &= 2\boldsymbol{r}_i(t) - \boldsymbol{r}_i(t-\delta t) + \ddot{\boldsymbol{r}}_i(t)(\delta t)^2 + \frac{2}{4!}\ddddot{\boldsymbol{r}}_i(t)(\delta t)^4 + \ldots \\ &\approx 2\boldsymbol{r}_i(t) - \boldsymbol{r}_i(t-\Delta t) + \ddot{\boldsymbol{r}}_i(t)(\Delta t)^2 \end{aligned}$$

The required acceleration of the ith atom is calculated from the conservative force $\boldsymbol{F}_i$, the atomic mass m_i, and, if $T \neq 0$, a thermodynamic friction coefficient $\xi(t)$. The force is obtained as a derivative of the respective potential. The velocity of the atom is calculated by subtracting equation (4.47) from equation (4.48).

$$\dot{\boldsymbol{r}}_i(t) \approx \frac{\boldsymbol{r}_i(t+\Delta t) - \boldsymbol{r}_i(t-\Delta t)}{2\Delta t}$$

Derived quantities

temperature

$$T(t) = \frac{2E_{\mathrm{kin}}}{3Nk_{\mathrm{B}}} = \frac{1}{3Nk_{\mathrm{B}}} \sum_{i=1}^{N} m_i v_i^{\;2}(t)$$

pressure

$$P(t) = \frac{1}{3V} \sum_{i=1}^{N} \left(m_i v_i^2 + r_i F_i \right)$$

Derived quantities

Spezific heat

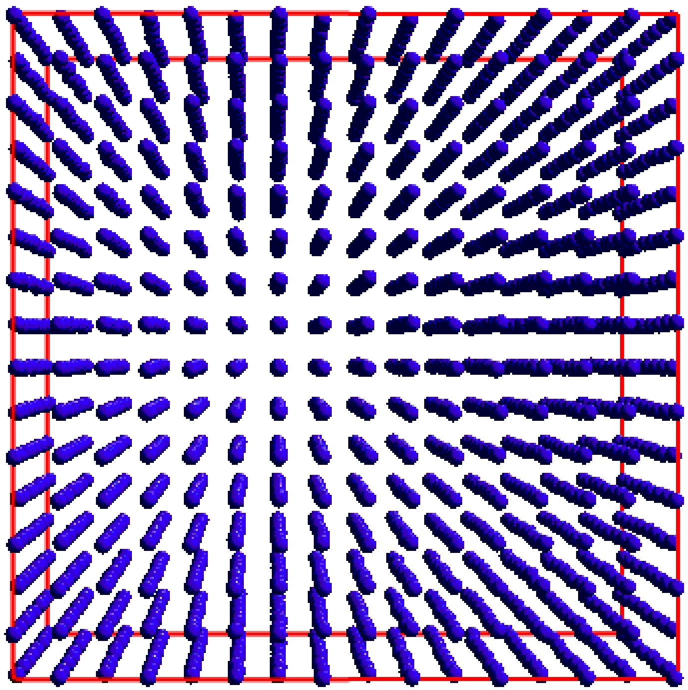
$$\frac{\langle T^2\rangle - \langle T\rangle^2}{\langle T\rangle^2} = \frac{2}{3N}\left(1 - \frac{3k_\mathrm{B}N}{2C_v}\right)$$

Diffusion constant

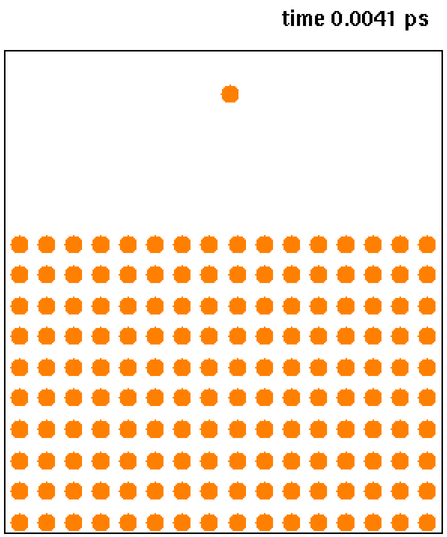
$$D(t) = \frac{1}{6t}\left\langle \left(r_i(\tau+t) - r_i(\tau)\right)^2 \right\rangle$$

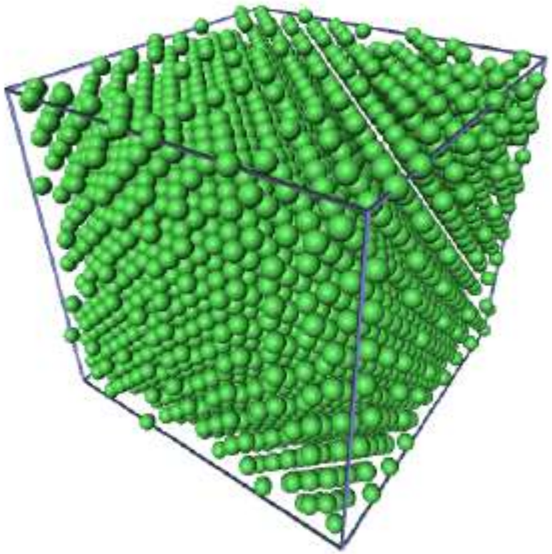
pair correlation

$$g(r) = \frac{V}{4\pi N^2 r^2}\left\langle \left(\sum_i \sum_{i\neq j} \delta(r - r_{ij} \right) \right\rangle$$

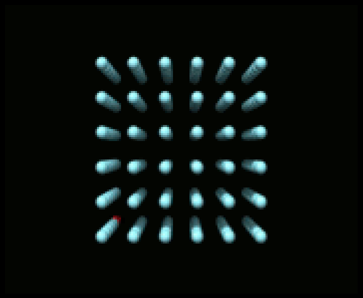


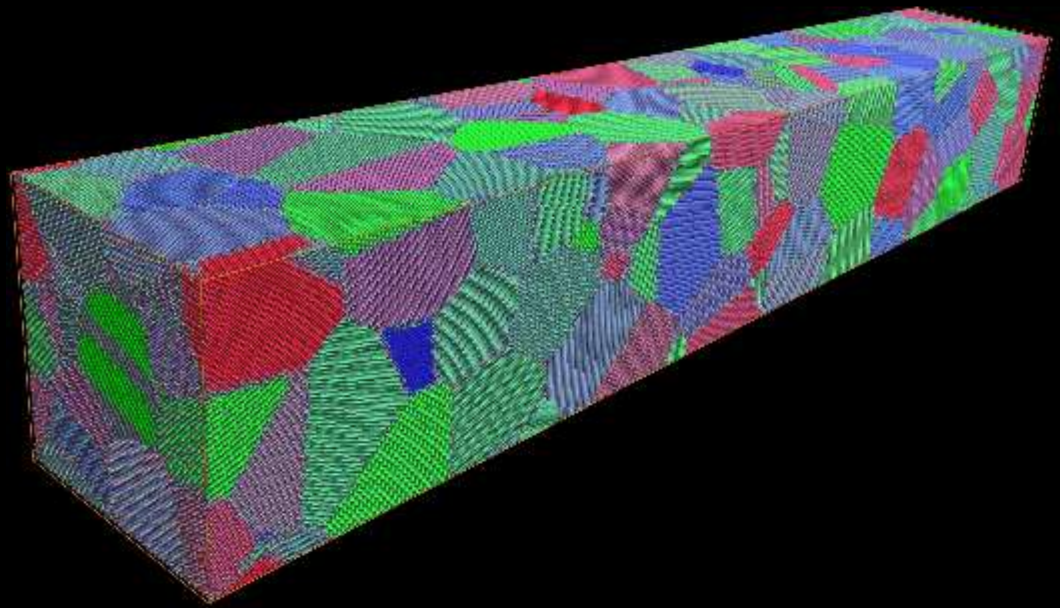
Molecular Dynamics

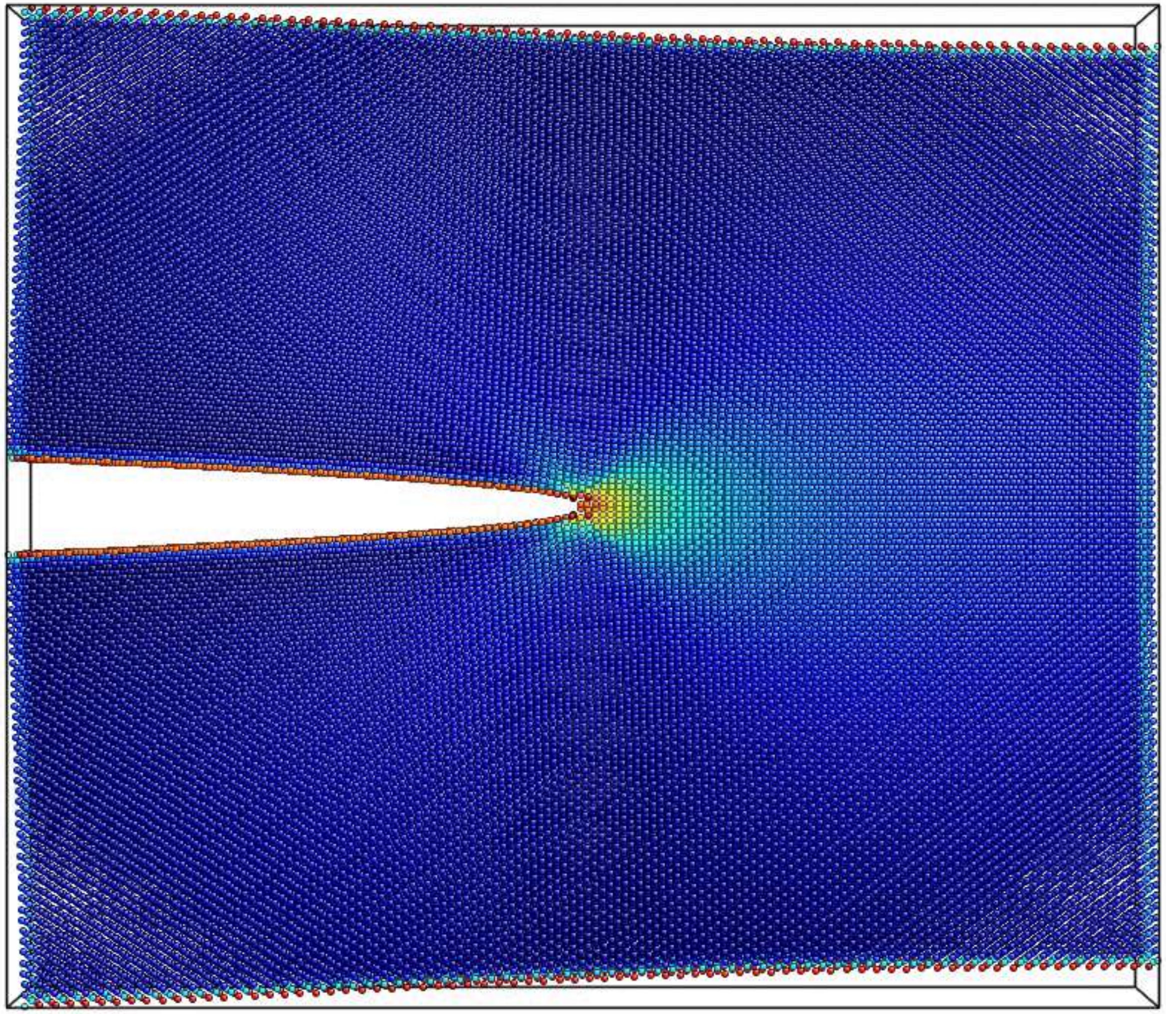




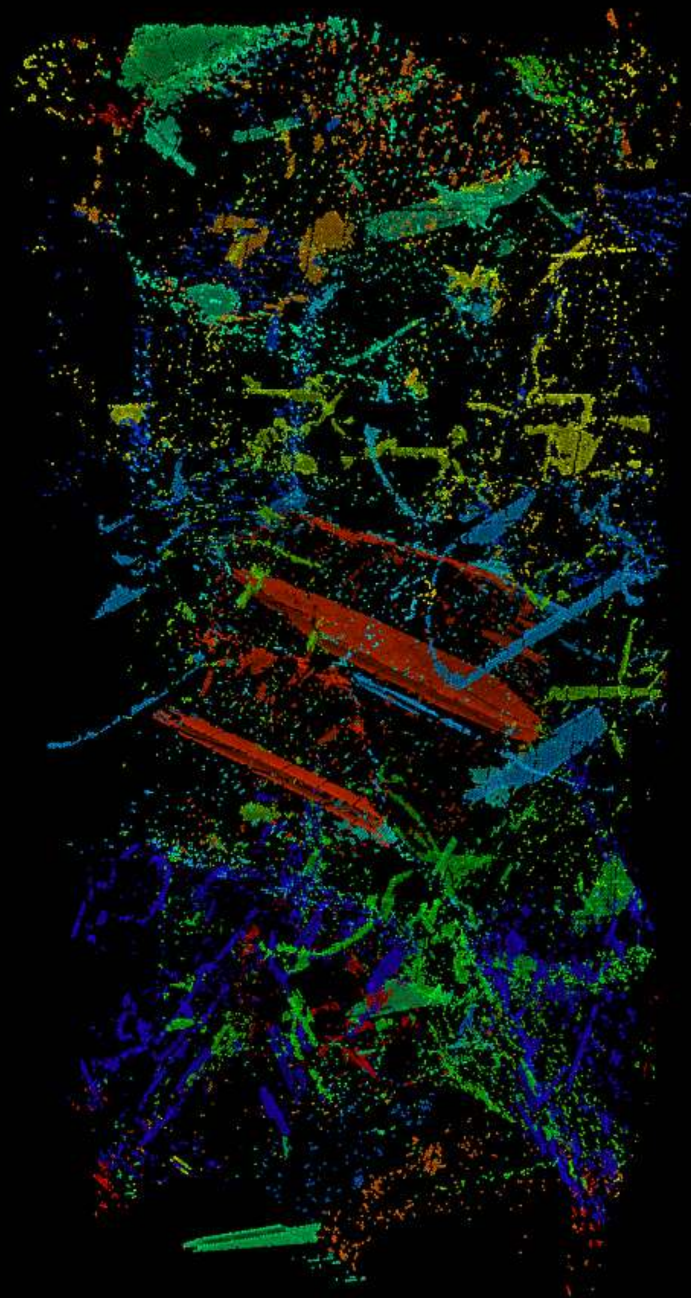
Molecular Dynamics







Postech CMSE Lab.



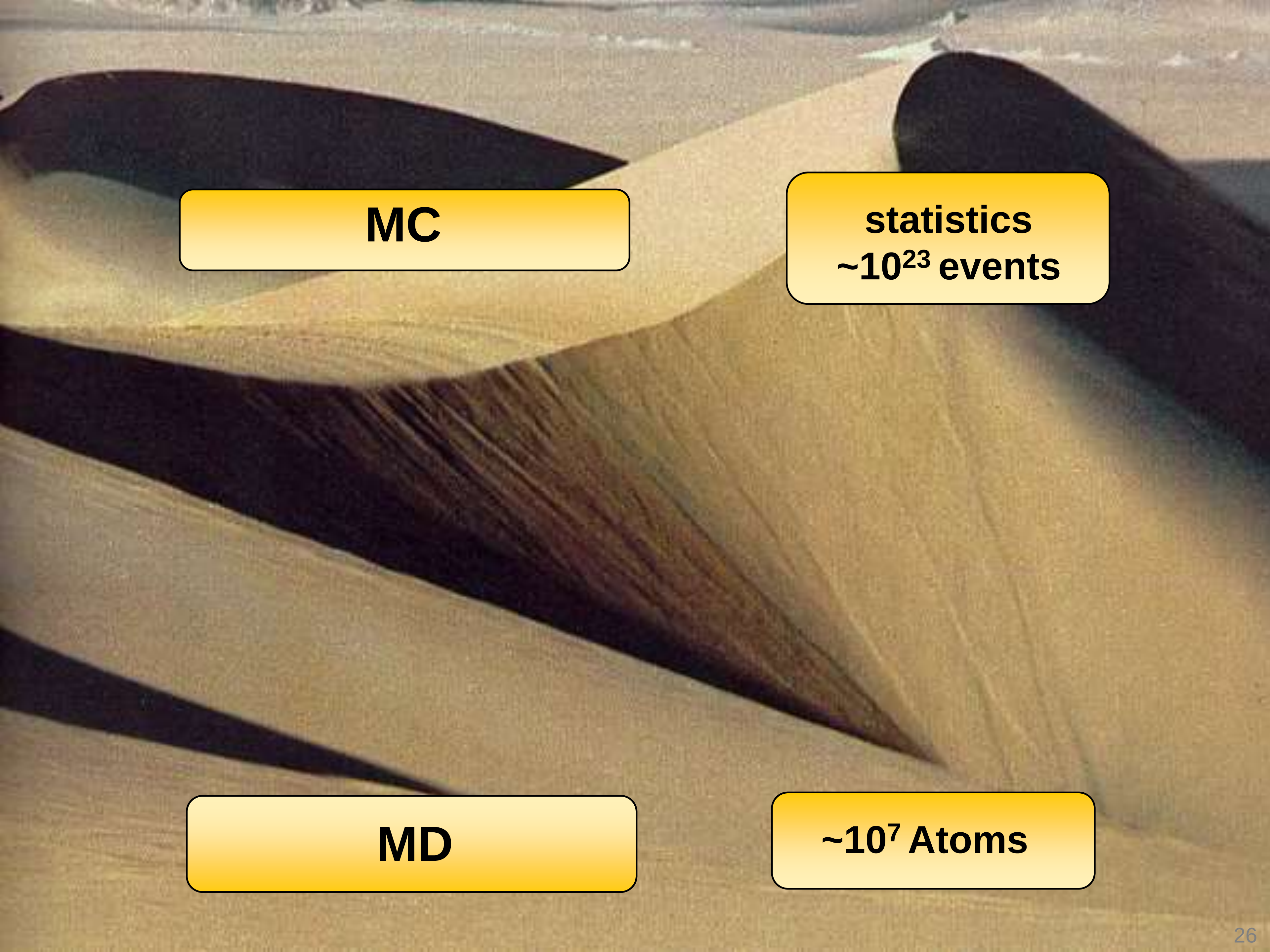
Gauss Centre for Supercomputing MD-Simulations on Strengthening Caused by GP-Zones in Al-Cu Alloys

Overview

- Some basic methods
  - Atomistic
  - Monte Carlo
  - Dislocations
  - Polycrystal mechanics

- Ab-initio informed constitutive models
  - Elasticity: from DFT to Homogenization
  - Atomistically informed simulation: from APT to MD
  - From DFT to dislocation rate models and yield surfaces

DFT: Density Functional Theory; APT: Atom Probe Tomography; MD: Molecular Dynamics; RVE: Representative Volume Element; ICME: Integrated Computational Materials Engineering



MC

statistics
~10^{23} events

MD

~10^{7} Atoms

Algorithms that use sequence of random events

Average behavior (statistics)

Kinetics: e.g. diffusion such as random walk (drunken sailor)

Thermodynamics: Phase transitions (Ising and Potts Models)

General

Formulate a probabilistic analogue of the problem

Apply a Monte Carlo algorithm

Present and interpret results

Mathematical

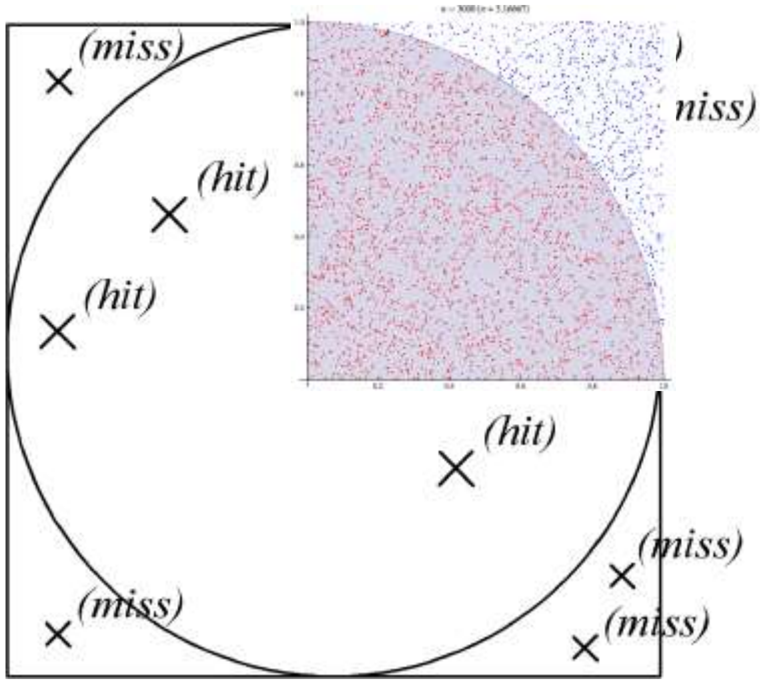
Formulate integral expressions of the governing differential equations that describe the stochastic process

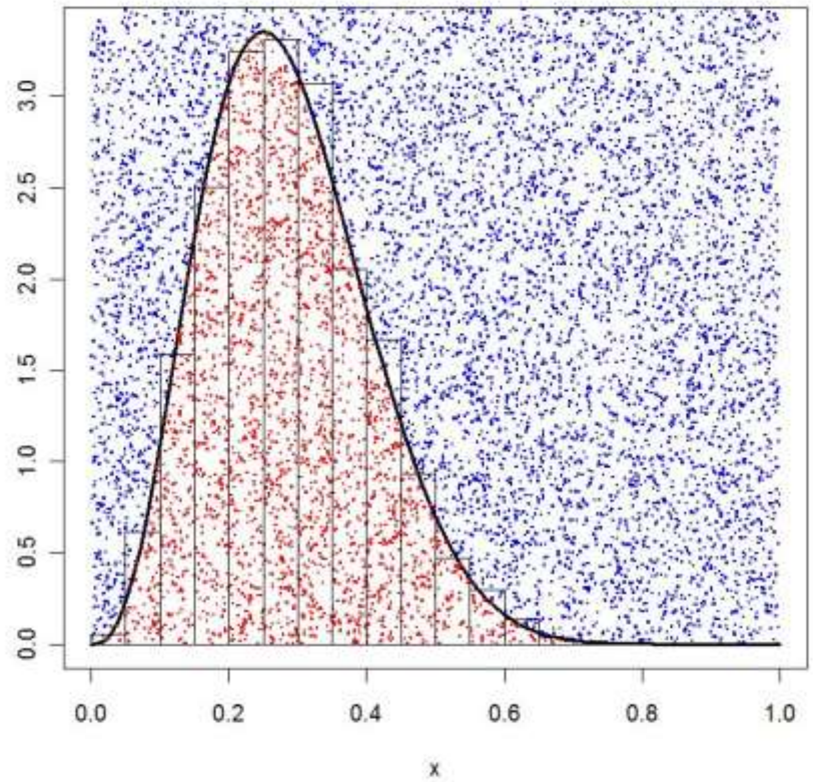
Integrate the governing expression using a weighted or nonweighted random sampling method

Extract state equation values, correlation functions, structural information, or MC kinetics

Numerical integration using random numbers (stochastic integration)

e.g. circle area





$$\frac{\text{circle area}}{\text{square area}} = \frac{\pi r^2}{(2r)^2} = \frac{\pi}{4} = \frac{n_{\text{Treffer}}}{n_{\text{ges}}}$$

Monte Carlo

Problem: $$\langle A \rangle = \int P(X) A(X) dX$$

$$mit \quad P(X) = \frac{1}{Z} \exp\left(-\frac{H(X)}{k_B T} \right)$$

Numerical Integration:

$$\langle A \rangle \approx \overline{A} = \frac{1}{M} \sum_{i=1}^{M} P(X_i) A(X_i), \quad M \to \infty$$

BUT: phase space very large
Solution: importance sampling

Metropolis Algorithm: importance sampling: prescribe areas where it is worth to look ! (meaning where to integrate)

create sequence of states $X_\nu \rightarrow X_{\nu+1} \rightarrow X_{\upsilon+2} \rightarrow \ldots$

using transition probability $W(X \rightarrow X')$

e.g.: $\Delta H = H(X') - H(X)$

$$W(X \rightarrow X') = \begin{cases} 1 & if \;\; \Delta H \leq 0 \\ \exp(-\Delta H / k_B T) & if \;\; \Delta H > 0 \end{cases}$$

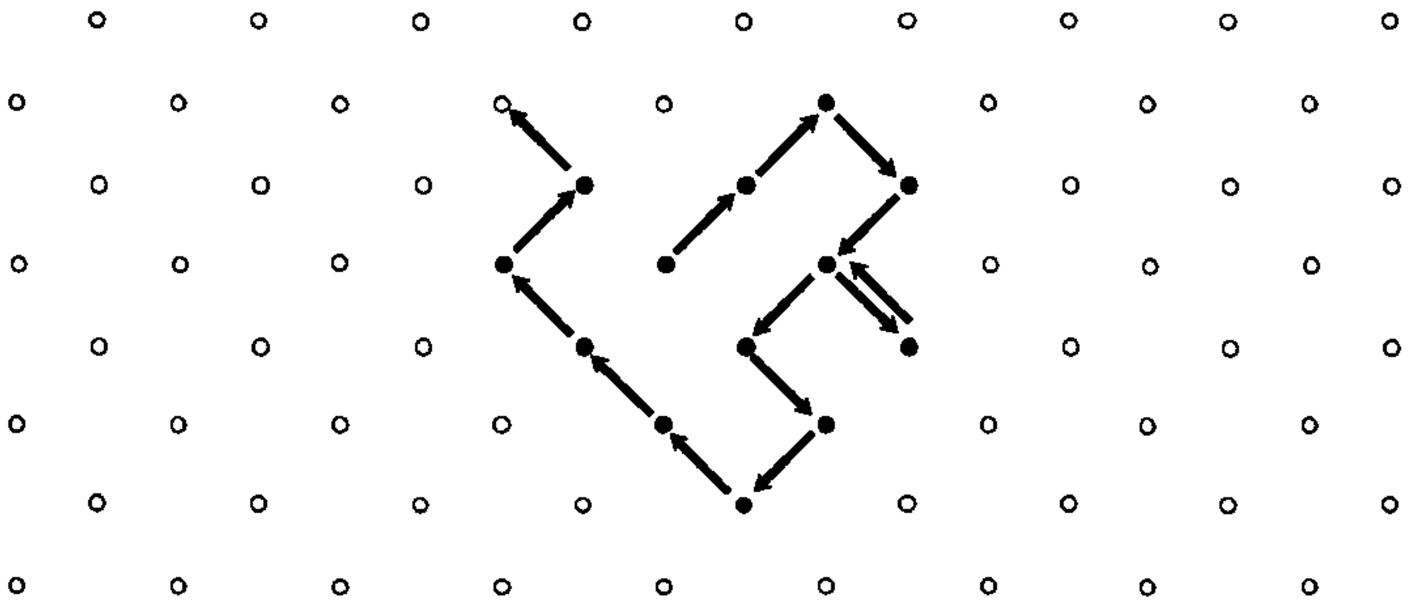
W fulfills condition of detailed balance

$$P(X)W(X \rightarrow X') = P(X')W(X' \rightarrow X)$$

and hence

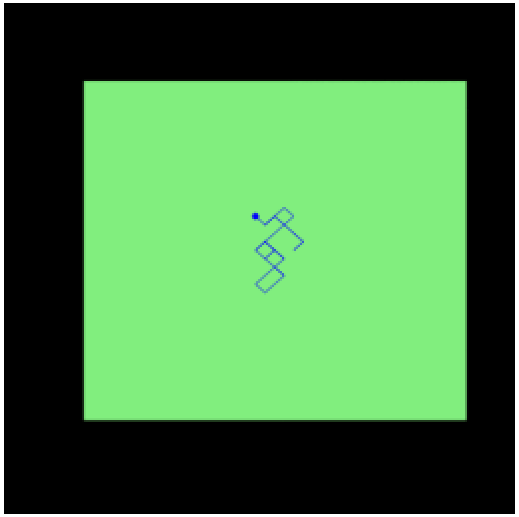
$$\overline{A} = \frac{1}{M}\sum_{i=1}^{M} A(X_i)$$

Monte Carlo: diffusion

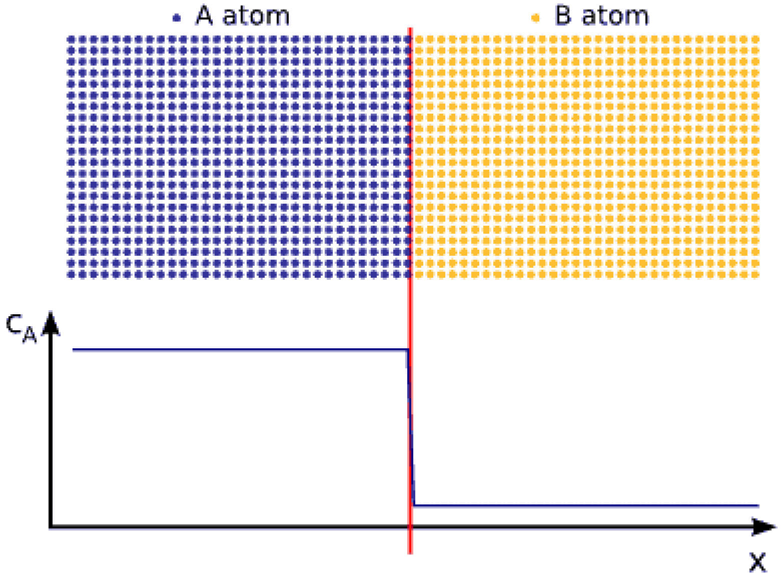


$$x^2 = 6D\tau$$

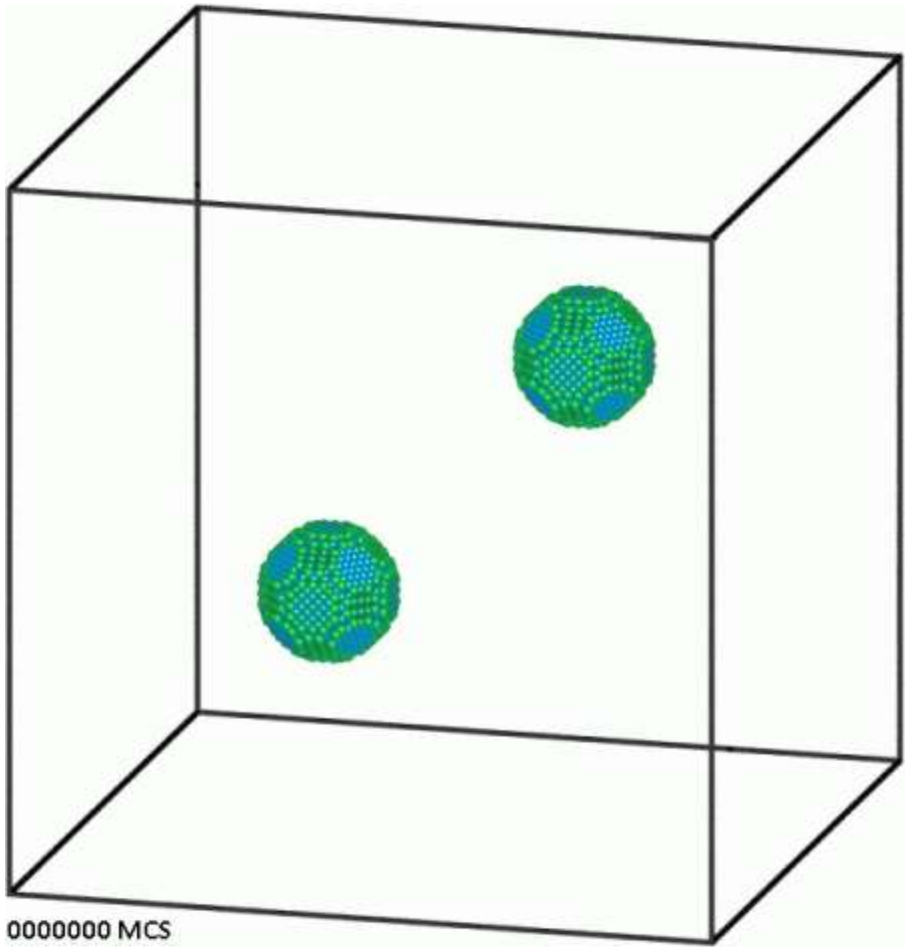
$$\Delta x \propto \sqrt{\tau}$$



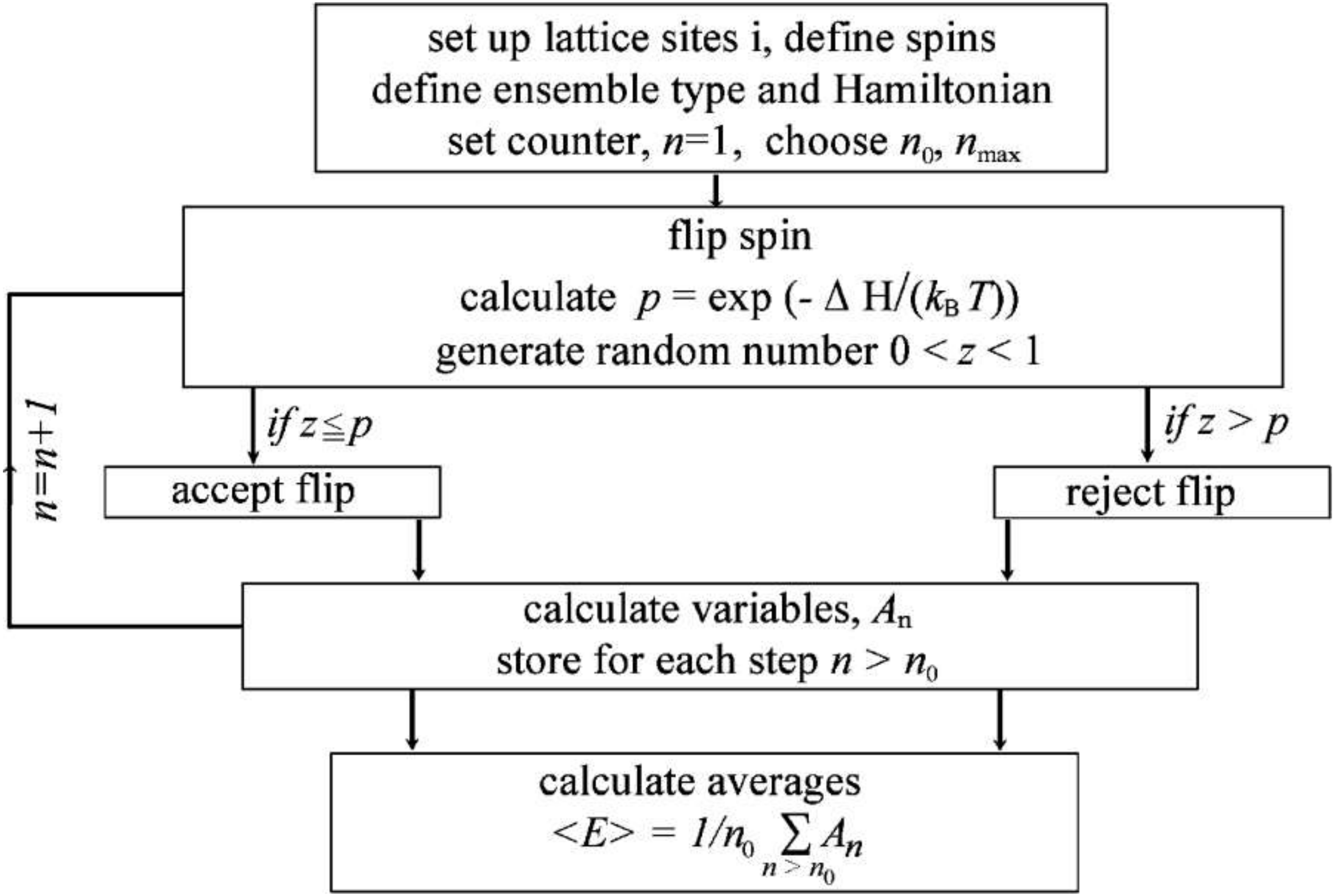
Monte Carlo: diffusion

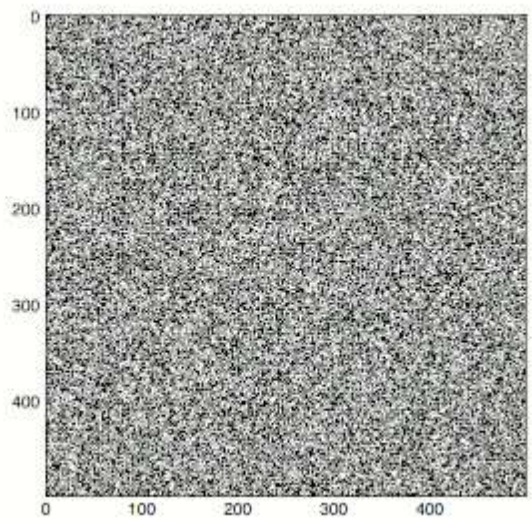


Monte Carlo: Coarsening

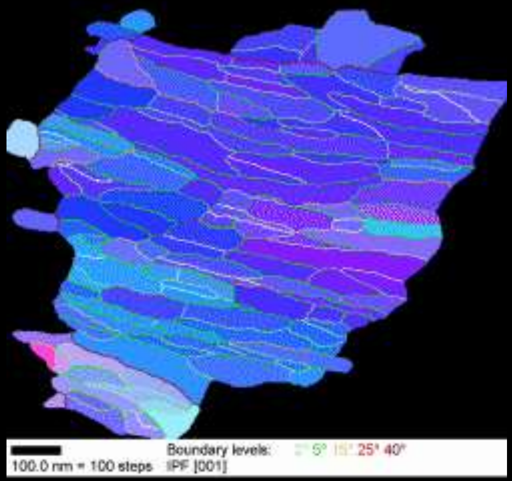


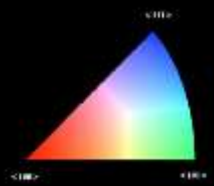
Monte Carlo Ising and Potts models

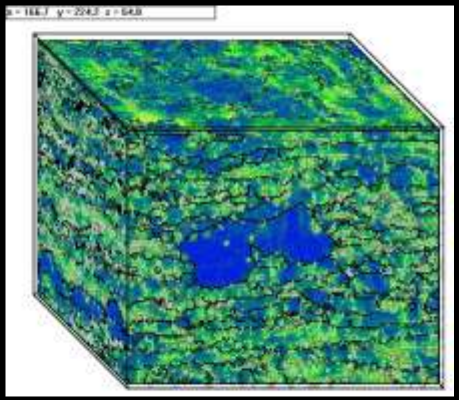


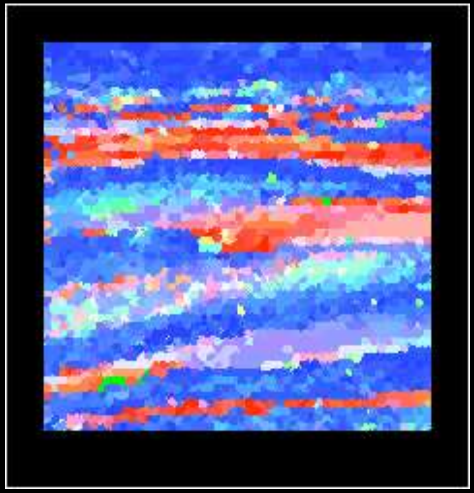

0
100
200
300
400
0
100
200
300
400

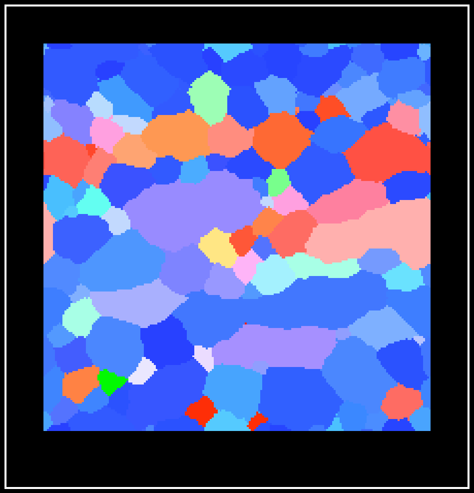
Monte Carlo: Potts model

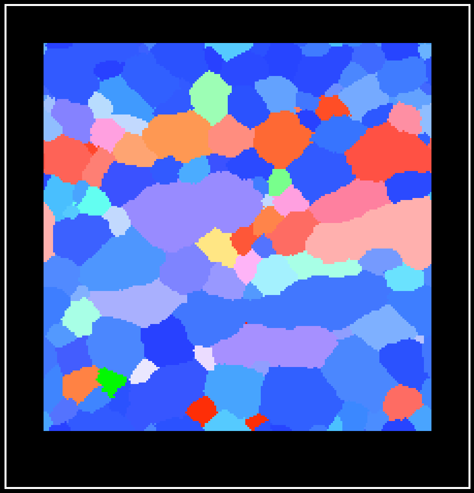












S. Zaefferer, Y. Chen

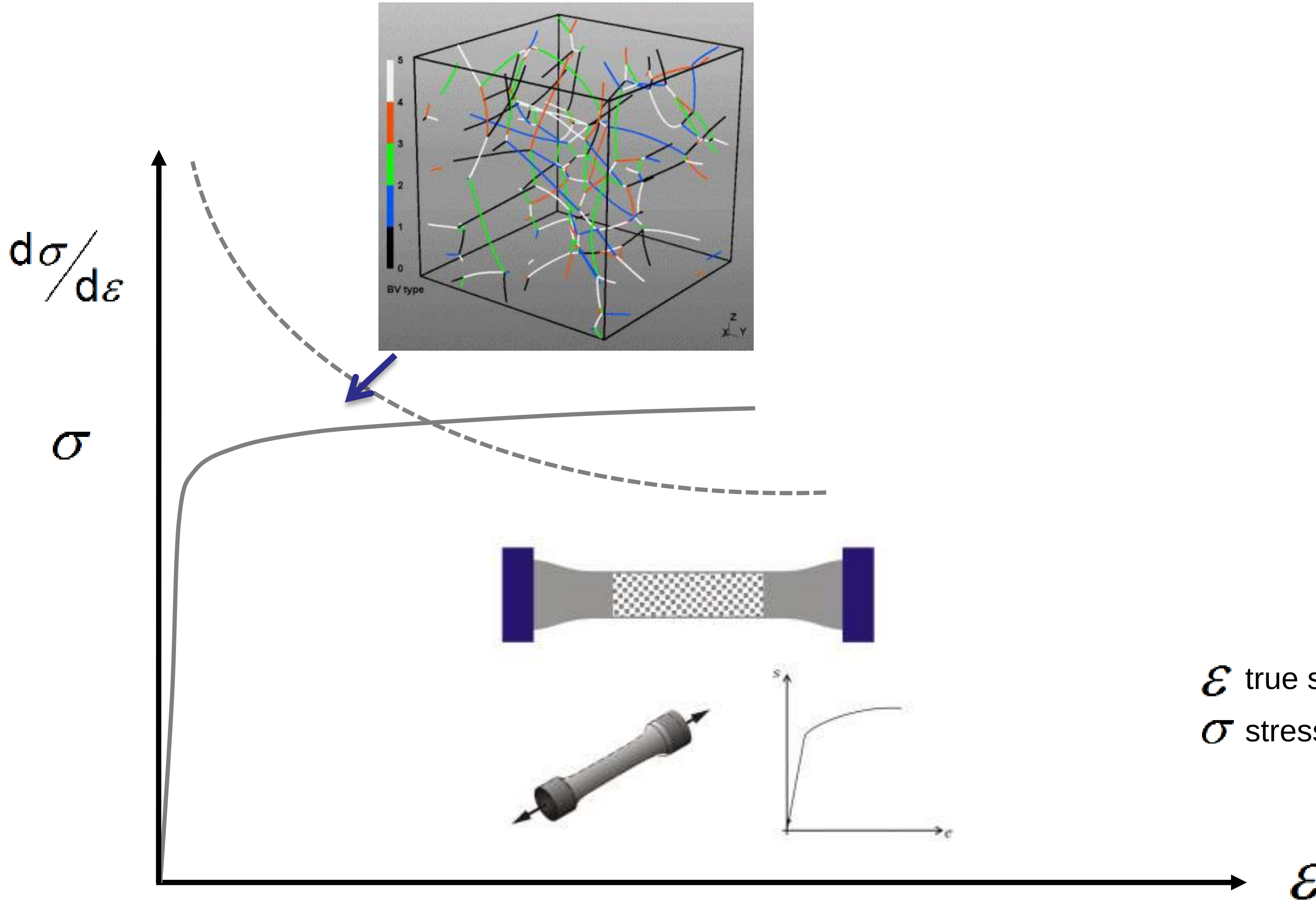
Overview

- Some basic methods
  - Atomistic
  - Monte Carlo
  - Dislocations
  - Polycrystal mechanics

- Ab-initio informed constitutive models
  - Elasticity: from DFT to Homogenization
  - Atomistically informed simulation: from APT to MD
  - From DFT to dislocation rate models and yield surfaces

DFT: Density Functional Theory; APT: Atom Probe Tomography; MD: Molecular Dynamics; RVE: Representative Volume Element; ICME: Integrated Computational Materials Engineering

Dislocations and strain hardening



ε true strain

σ stress

Kinematics: displacement vector in continuum space

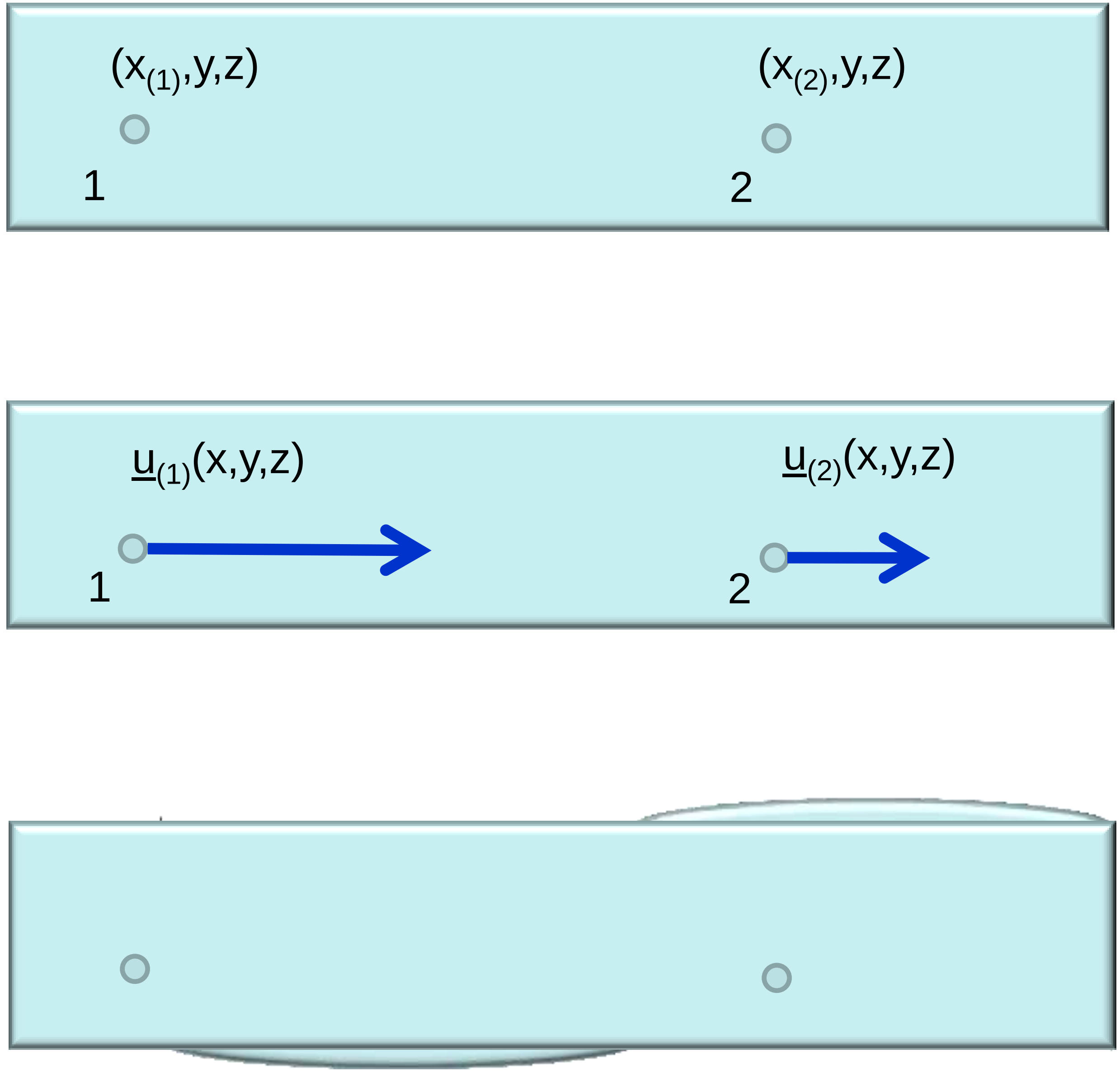
$\underline{u}=u(x,y,z)$

$\underline{u}_{(1)}(x,y,z)=\underline{u}_{(2)}(x,y,z)$

Kinematics: displacement vector in continuum space

$\underline{u}=u(x,y,z)$

$\underline{u}_{(1)}(x,y,z)\neq\underline{u}_{(2)}(x,y,z)$



Kinematics, displacement, displacement gradient: general

Distorsions come from gradients in the displacement fields

Displacement vector:

$$\mathbf{u} = [u_x, u_y, u_z]$$

Strain tensor:

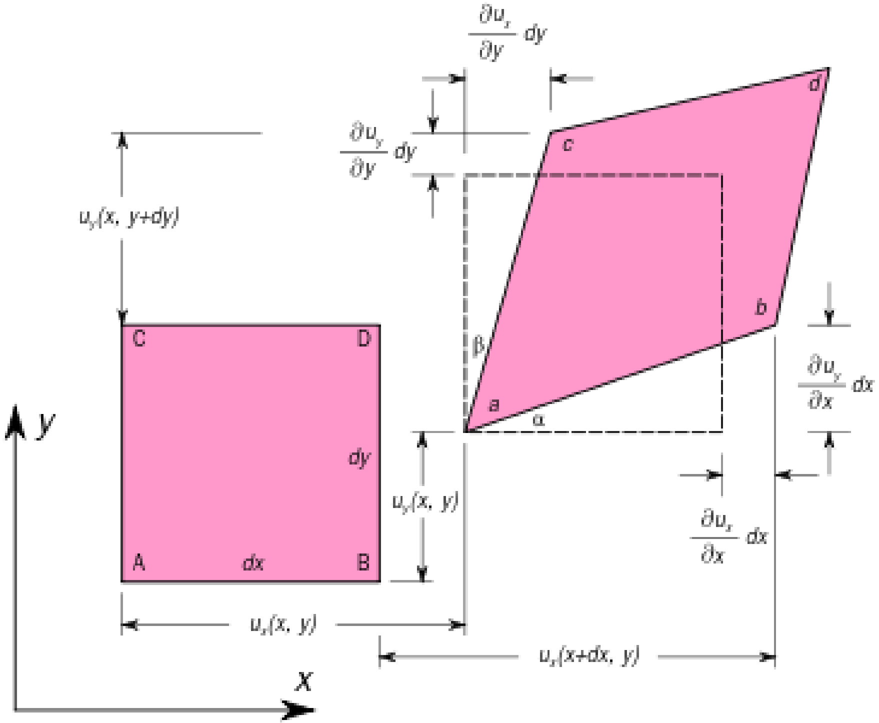
$$\varepsilon_{xx} = \frac{\partial u_x}{\partial x}$$

Strain tensor: symmetrical part of displacement gradient tensor

Displacement gradient

The tensor $\frac{\partial u_i}{\partial x_j}$ is called **displacement gradient tensor** and may be written as

$$\frac{\partial u_i}{\partial x_j} = u_{i,j} = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} & \frac{\partial u}{\partial z} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} & \frac{\partial v}{\partial z} \\ \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} & \frac{\partial w}{\partial z} \end{bmatrix}$$



Displacement gradient tensor

The displacement gradient tensor in general is a non-symmetric tensor and can be decomposed into symmetric and antisymmetric part. Hence the displacement is

$$
\begin{aligned}
u_i &= \underbrace{u_i^0}_{\text{translation vector}} + \underbrace{\frac{1}{2}\left(u_{i,j} + u_{j,i}\right)}_{\text{strain tensor}} \mathrm{d}x_j + \underbrace{\frac{1}{2}\left(u_{i,j} - u_{j,i}\right)}_{\text{rotation tensor}} \mathrm{d}x_j \\
&= u_i^0 + \varepsilon_{ij}\mathrm{d}x_j + \omega_{ij}\mathrm{d}x_j
\end{aligned}
$$

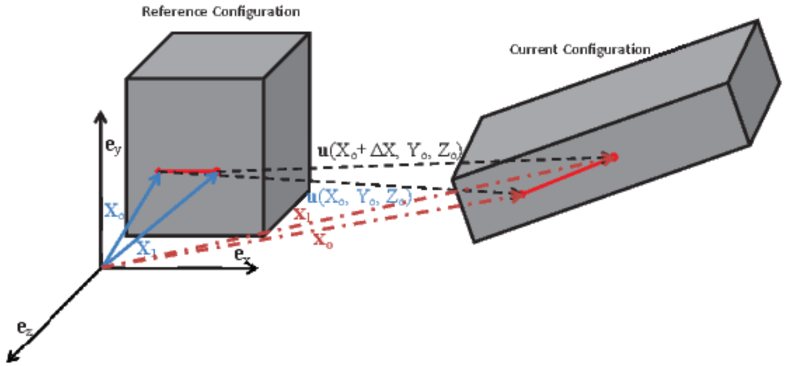
Displacement gradient tensor

Matrix expression of the strain tensor

$$\varepsilon = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{xy} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{xz} & \varepsilon_{yz} & \varepsilon_{zz} \end{bmatrix}$$

Matrix expression of the rotation tensor

$$\omega = \begin{bmatrix} 0 & \omega_{xy} & \omega_{xz} \\ -\omega_{xy} & 0 & \omega_{yz} \\ -\omega_{xz} & -\omega_{yz} & 0 \end{bmatrix}$$

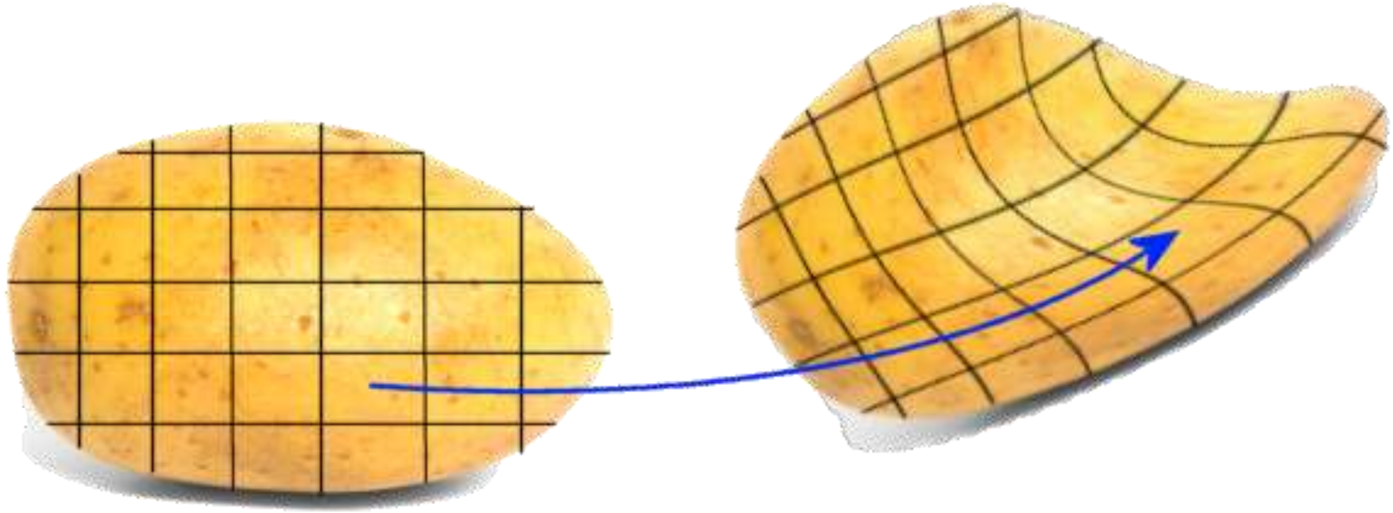


strain rates and displacement gradients in crystals

$$\dot{\varepsilon}_{ij}^{K} = D_{ij}^{K} = \frac{1}{2}\left(\dot{u}_{i,j}^{\mathrm{K}} + \dot{u}_{j,i}^{\mathrm{K}}\right) = \sum_{s=1}^{N} m_{ij}^{\mathrm{sym},s}\,\dot{\gamma}^{s} \qquad \text{mit} \qquad m_{ij}^{\mathrm{sym}} = m_{ji}^{\mathrm{sym}} = \frac{1}{2}\left(n_i b_j + n_j b_i\right)$$

plastic spin from polar decomposition

$$\dot{\omega}_{ij}^{K} = W_{ij}^{K} = \frac{1}{2}\left(\dot{u}_{i,j}^{\mathrm{K}} - \dot{u}_{j,i}^{\mathrm{K}}\right) = \sum_{s=1}^{N} m_{ij}^{\mathrm{asym},s}\,\dot{\gamma}^{s} \qquad \text{mit} \qquad m_{ij}^{\mathrm{asym}} = -m_{ji}^{\mathrm{asym}} = \frac{1}{2}\left(n_i b_j - n_j b_i\right)$$



Displacement gradient tensor: the Cauchy strain

Strain tensor

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right)$$

In matrix form

$$\varepsilon = \frac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right)$$

The above strain tensor is called **Caushy strain tensor**

Displacement gradient tensor: the Cauchy strain

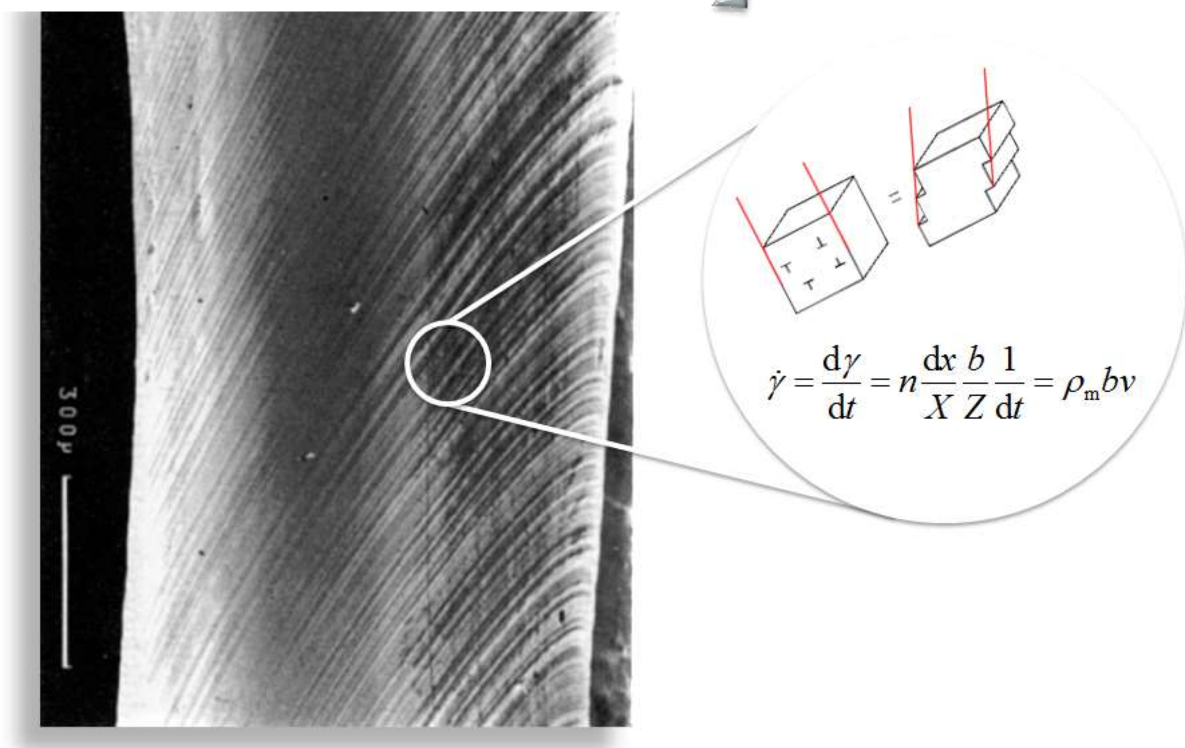
$$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right)$$

$$= \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\partial u_1}{\partial x_1} & \frac{1}{2}\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right) & \frac{1}{2}\left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right) \\ \frac{1}{2}\left(\frac{\partial u_2}{\partial x_1} + \frac{\partial u_1}{\partial x_2}\right) & \frac{\partial u_2}{\partial x_2} & \frac{1}{2}\left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}\right) \\ \frac{1}{2}\left(\frac{\partial u_3}{\partial x_1} + \frac{\partial u_1}{\partial x_3}\right) & \frac{1}{2}\left(\frac{\partial u_3}{\partial x_2} + \frac{\partial u_2}{\partial x_3}\right) & \frac{\partial u_3}{\partial x_3} \end{bmatrix}$$

strain rates and displacement gradients in crystals

$$\dot{\varepsilon}_{ij}^{K} = D_{ij}^{K} = \frac{1}{2}\left(\dot{u}_{i,j}^{\mathrm{K}} + \dot{u}_{j,i}^{\mathrm{K}}\right) = \sum_{s=1}^{N} m_{ij}^{\mathrm{sym},s}\dot{\gamma}^{s} \qquad \text{mit} \qquad m_{ij}^{\mathrm{sym}} = m_{ji}^{\mathrm{sym}} = \frac{1}{2}\left(n_i b_j + n_j b_i\right)$$



$$\dot{\gamma} = \frac{\mathrm{d}\gamma}{\mathrm{d}t} = n\frac{\mathrm{d}x}{X}\frac{b}{Z}\frac{1}{\mathrm{d}t} = \rho_{\mathrm{m}} b v$$

Displacement gradient tensor: strain components

Normal strains

$$\varepsilon_{xx} = \frac{\partial u}{\partial x}, \quad \varepsilon_{yy} = \frac{\partial v}{\partial y}, \quad \varepsilon_{zz} = \frac{\partial w}{\partial z}$$

Shear strains

$$\varepsilon_{xy} = \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)$$

$$\varepsilon_{xz} = \frac{1}{2}\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)$$

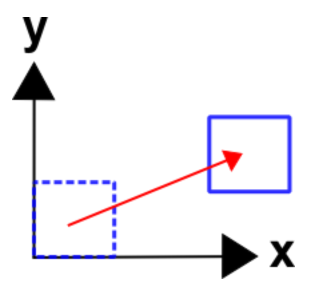
$$\varepsilon_{yz} = \frac{1}{2}\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)$$

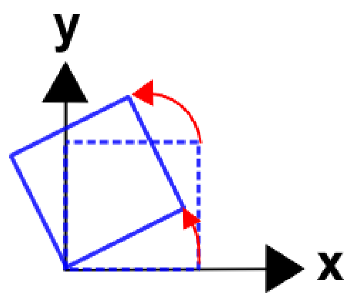
Engineering shear strains

$$\gamma_{xy} = 2\varepsilon_{xy}, \quad \gamma_{xz} = 2\varepsilon_{xz}, \quad \gamma_{yz} = 2\varepsilon_{yz}$$

Displacement gradient tensor: special cases

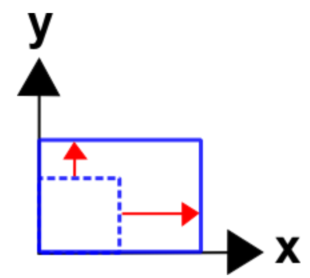
Rigid Body Displacements

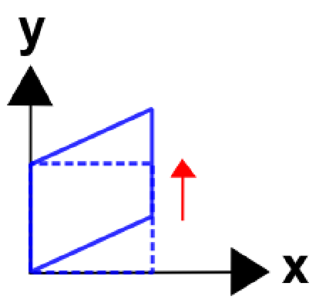




Rigid Body Rotations

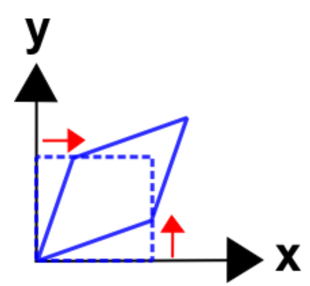
Stretching



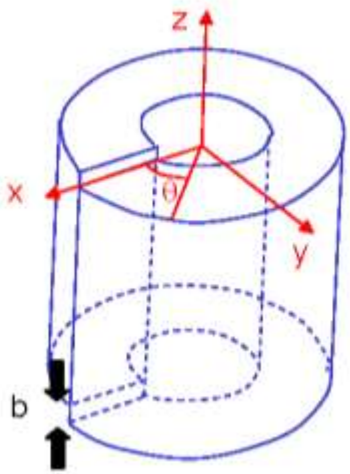


Shear (with Rotation)

Pure Shear



Displacement and strain field: infinite straight screw dislocation



"Recipe" :
- take a hollow cylinder, axis along z;
- cut on a plane parallel to the z-axis;
-displace the free surfaces by **b** in the z-direction.

By inspection:

$$u_x = u_y = 0$$

$$u_z = \frac{b\theta}{2\pi} = \frac{b}{2\pi}\tan^{-1}\left(\frac{y}{x}\right)$$

$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = \varepsilon_{xy} = \varepsilon_{yx} = 0$$

$$\varepsilon_{xz} = \tfrac{1}{2}\frac{\partial u_z}{\partial x} = \frac{b}{4\pi}\frac{\partial}{\partial x}\tan^{-1}\left(\frac{y}{x}\right) = -\frac{b}{4\pi}\frac{1}{1+\left(y/x\right)^2}\frac{y}{x^2} = -\frac{b}{4\pi}\frac{y}{x^2+y^2} = -\frac{b}{4\pi}\frac{\sin\theta}{r}$$

$$\varepsilon_{yz} = \tfrac{1}{2}\frac{\partial u_z}{\partial y} = \frac{b}{4\pi}\frac{\partial}{\partial y}\tan^{-1}\left(\frac{y}{x}\right) = \frac{b}{4\pi}\frac{1}{1+\left(y/x\right)^2}\frac{1}{x} = \frac{b}{4\pi}\frac{x}{x^2+y^2} = \frac{b}{4\pi}\frac{\cos\theta}{r}$$

Stress field of straight screw dislocation

$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = \varepsilon_{xy} = \varepsilon_{yx} = 0$$

$$\varepsilon_{xz} = -\frac{b}{4\pi}\frac{y}{x^2+y^2} = -\frac{b}{4\pi}\frac{\sin\theta}{r}$$

$$\varepsilon_{yz} = \frac{b}{4\pi}\frac{x}{x^2+y^2} = \frac{b}{4\pi}\frac{\cos\theta}{r}$$

$$\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = \sigma_{xy} = \sigma_{yx} = 0$$

$$\Delta = 0$$

$$\sigma_{xz} = 2G\varepsilon_{xz} = -\frac{Gb}{2\pi}\frac{y}{x^2+y^2} = -\frac{Gb}{2\pi}\frac{\sin\theta}{r}$$

$$\sigma_{yz} = 2G\varepsilon_{yz} = \frac{Gb}{2\pi}\frac{x}{x^2+y^2} = \frac{Gb}{2\pi}\frac{\cos\theta}{r}$$

In Polar coordinates:

(either by direct inspection, or by transforming the strains and stresses from Cartesian co-ordinates)

$$\varepsilon_{\theta z} = \varepsilon_{z\theta} = \frac{b}{4\pi r}$$

$$\sigma_{\theta z} = \sigma_{z\theta} = \frac{Gb}{2\pi r}$$

All other components of the stress tensor are zero.

Note:
- Stress and strain fields are pure shear
- Fields have radial symmetry
- Stresses and strains are proportional to 1/r:
  - extend to infinity
  - tend to infinite values as $r \Rightarrow 0$

Infinite stresses cannot exist in real materials: the dislocation core radius r_0 is that within which our assumption of linear elastic behaviour breaks down. Typically $r_0 \approx 1$ nm.

Summary: infinite straight screw dislocation

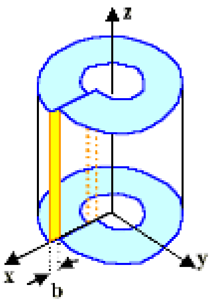
$$\underline{u}(\underline{x}) = \begin{pmatrix} 0 \\ 0 \\ \frac{b}{2\pi} \arctan \frac{y}{x} \end{pmatrix}$$

$$\underline{\underline{\varepsilon}}(\underline{x}) = \begin{pmatrix} 0 & 0 & -\frac{b}{4\pi}\frac{y}{x^2+y^2} \\ 0 & 0 & \frac{b}{4\pi}\frac{x}{x^2+y^2} \\ -\frac{b}{4\pi}\frac{y}{x^2+y^2} & \frac{b}{4\pi}\frac{x}{x^2+y^2} & 0 \end{pmatrix}$$

$$\underline{\underline{\sigma}}(\underline{x}) = \frac{Gb}{2\pi} \begin{pmatrix} 0 & 0 & -\frac{b}{4\pi}\frac{y}{x^2+y^2} \\ 0 & 0 & \frac{b}{4\pi}\frac{x}{x^2+y^2} \\ -\frac{b}{4\pi}\frac{y}{x^2+y^2} & \frac{b}{4\pi}\frac{x}{x^2+y^2} & 0 \end{pmatrix}$$

Summary: infinite straight edge dislocation

$$
\begin{aligned}
u_x &= \frac{b}{2\pi}(\arctan\frac{y}{x} + \frac{1}{2(1-\nu)}\frac{xy}{x^2+y^2}) \\
u_y &= \frac{b}{2\pi}(-\frac{1-2\nu}{2(1-\nu)}\log\sqrt{x^2+y^2} + \frac{1}{2(1-\nu)}\frac{y^2}{x^2+y^2}) \\
u_z &= 0
\end{aligned}
$$



$$\varepsilon_{xx} = \frac{\partial u_x}{\partial x} = \frac{b\,y\,((3-2\,\nu)\,x^2 + (1-2\,\nu)\,y^2)}{4\,(-1+\nu)\,\pi\,(x^2+y^2)^2}$$

$$\varepsilon_{yy} = \frac{\partial u_y}{\partial y} = \frac{-(b\,y\,((1+2\,\nu)\,x^2 + (-1+2\,\nu)\,y^2))}{4\,(-1+\nu)\,\pi\,(x^2+y^2)^2}$$

$$\varepsilon_{xy} = \frac{1}{2}(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}) = \frac{b\,x\,(-x^2+y^2)}{4\,(-1+\nu)\,\pi\,(x^2+y^2)^2}$$

Summary: infinite straight edge dislocation

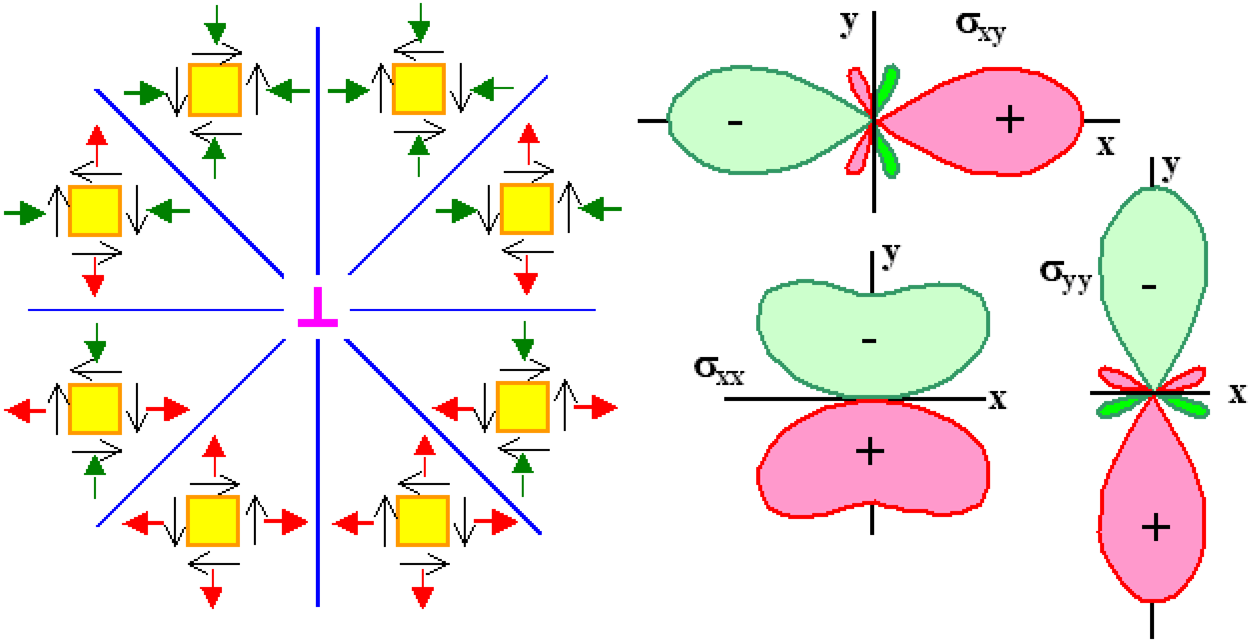
$$\sigma_{xx} = \frac{b\,G\,y\,(3\,x^2 + y^2)}{2\,(-1+\nu)\,\pi\,(x^2+y^2)^2}$$

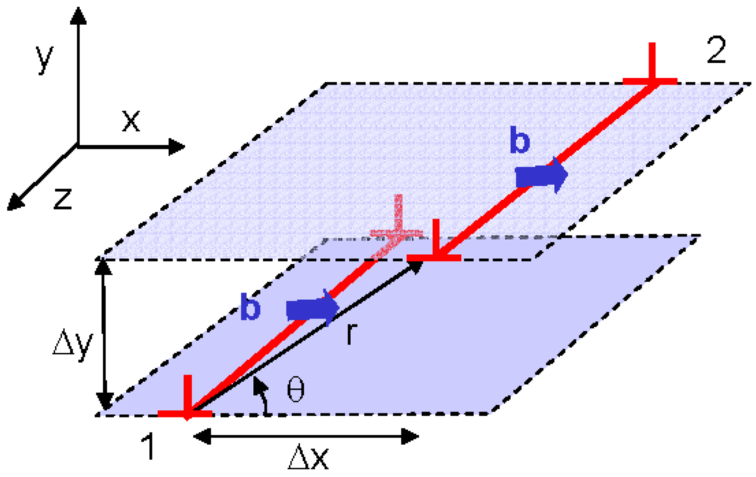
$$\sigma_{yy} = \frac{b\,G\,y\,(-x^2 + y^2)}{2\,(-1+\nu)\,\pi\,(x^2+y^2)^2}$$

$$\sigma_{zz} = \frac{b\,G\,\nu\,y}{(-1+\nu)\,\pi\,(x^2+y^2)}$$

$$\sigma_{xy} = \frac{b\,G\,x\,(-x^2 + y^2)}{2\,(-1+\nu)\,\pi\,(x^2+y^2)^2}$$

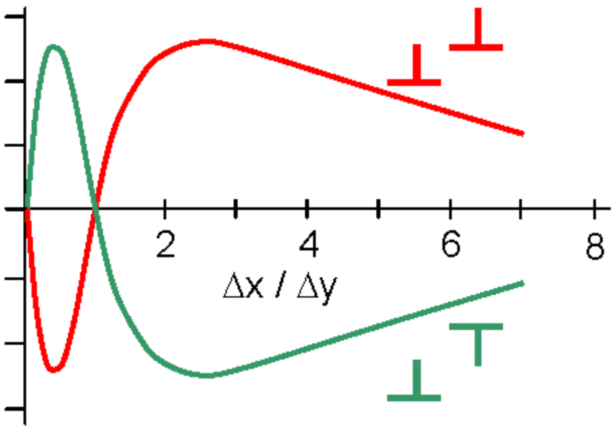
Forces and stress field: infinite straight edge dislocation





So glide force, resolved onto the slip plane, is:

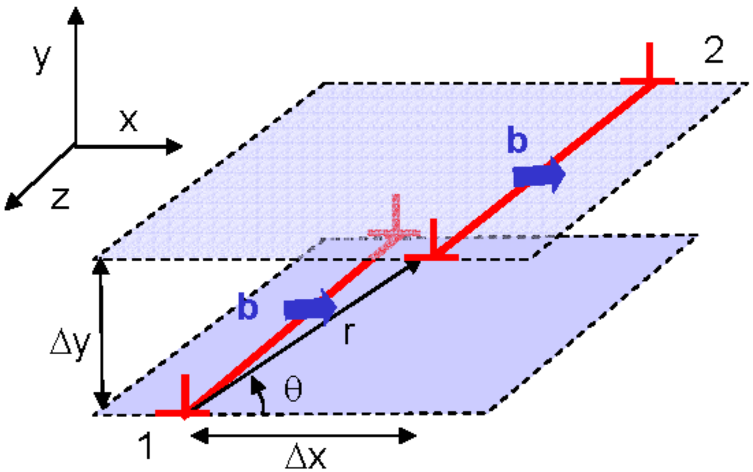
$$F_{glide} = \frac{Gb^2}{2\pi(1-\nu)} \frac{\Delta x(\Delta x^2 - \Delta y^2)}{\left(\Delta x^2 + \Delta y^2\right)^2}$$

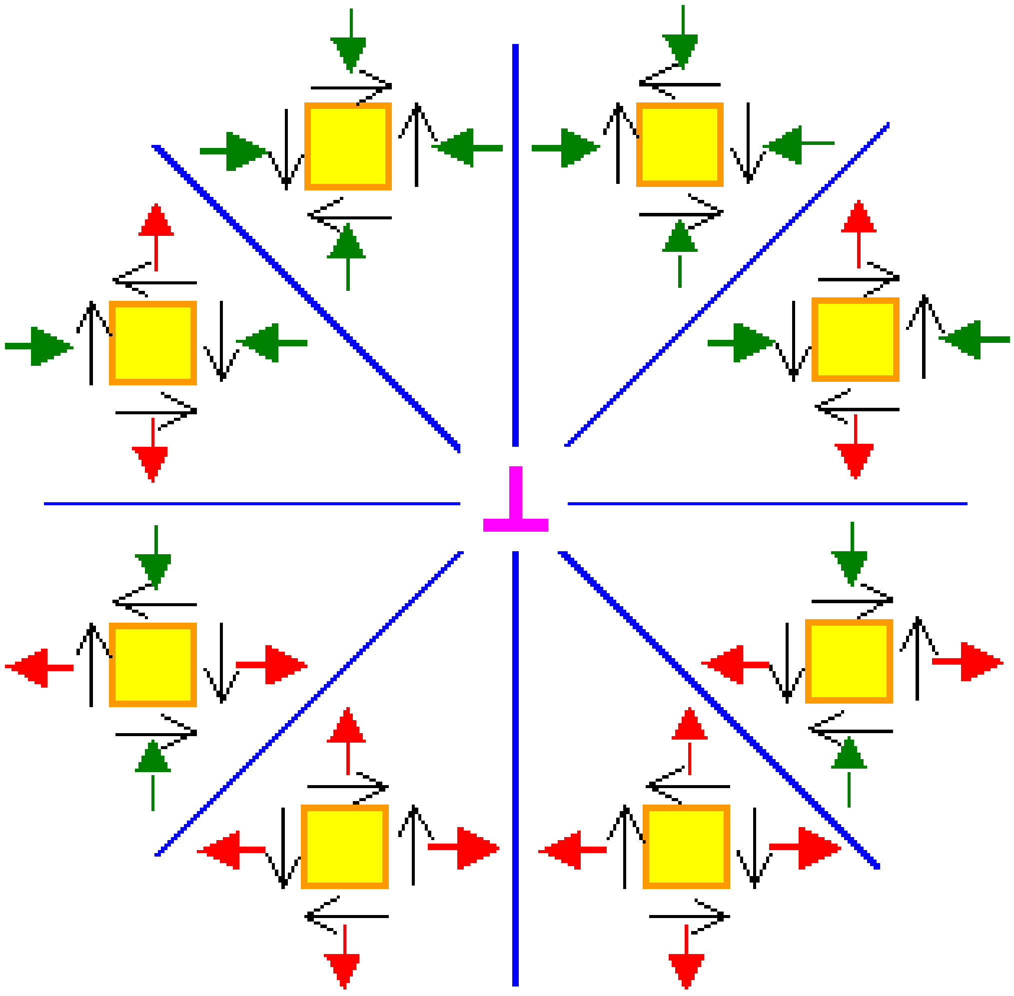


$$\frac{F_{glide}}{\frac{Gb^2}{2\pi(1-\nu)\Delta y}}$$

$$\sigma_{xx} = -D\,y\,\frac{3\Delta x^2 + \Delta y^2}{\left(\Delta x^2 + \Delta y^2\right)^2}, \qquad \text{with: } D = \frac{Gb}{2\pi(1-\nu)}$$

$$\sigma_{xy} = \sigma_{yx} = D\,\Delta x\,\frac{\Delta x^2 - \Delta y^2}{\left(\Delta x^2 + \Delta y^2\right)^2}$$

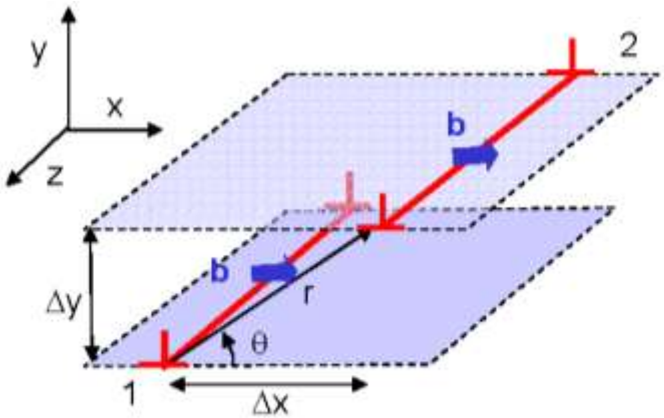




$$\sigma_{xx} = -D\,y\frac{3\Delta x^2 + \Delta y^2}{\left(\Delta x^2 + \Delta y^2\right)^2}, \quad \text{with: } D = \frac{Gb}{2\pi(1-\nu)}$$

$$\sigma_{xy} = \sigma_{yx} = D\,\Delta x\frac{\Delta x^2 - \Delta y^2}{\left(\Delta x^2 + \Delta y^2\right)^2}$$

Dynamics: forces among dislocations



Dislocation 2 "feels" the stress field of dislocation 1 (and vice versa).

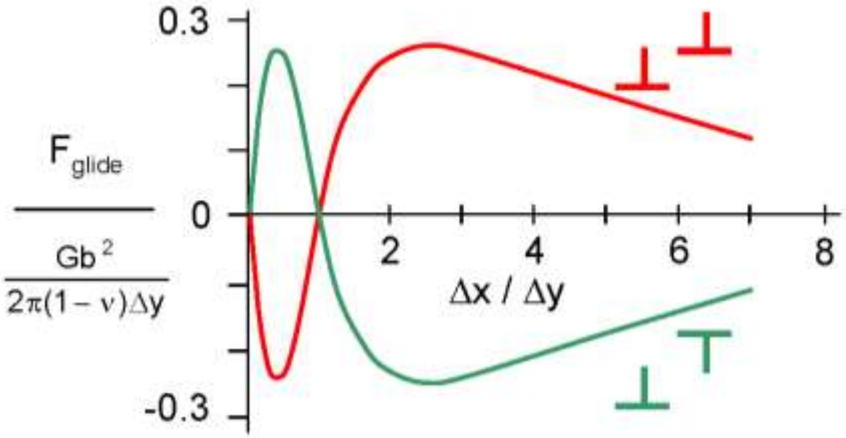
Peach-Koehler Force

$$\vec{F}_{1\to2} = \left(\underline{\underline{\sigma}}^{1\to2}\,\vec{b}_2\right)\times\vec{t}_2$$

σ_{xy} – produces *glide* force

σ_{xx} – produces *climb* force

Stable configurations for dislocation ensembles



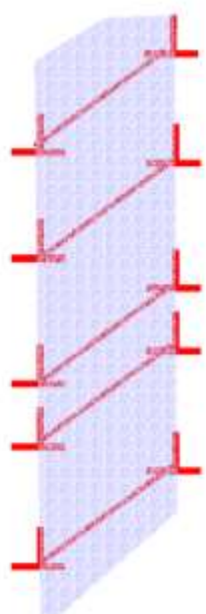
For **like** Burgers vectors:
Δx = ±Δy: unstable equilibrium
Δx = 0 : stable equilibrium

For **opposite** Burgers vectors:
Δx = ±Δy: stable equilibrium
Δx = 0 : unstable equilibrium

For **like** Burgers vectors:
Stable array is a planar stack

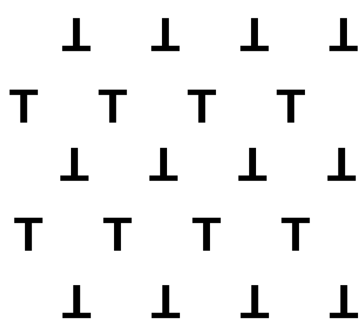
A low angle tilt boundary.

This arrangement has a strong long-range stress field.

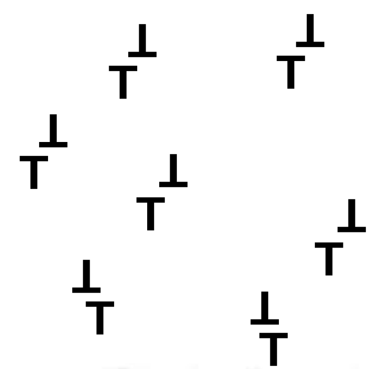


For a set of **“opposite”** Burgers vectors:

There are a large number of possible stable



“Taylor lattice”



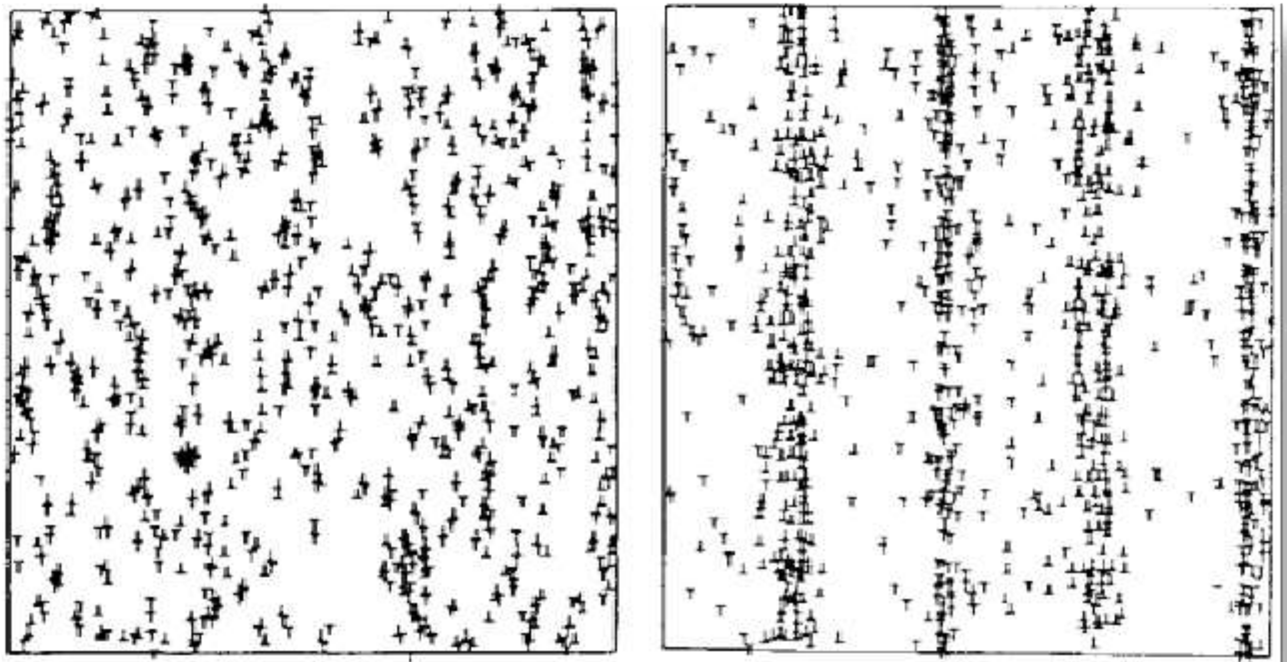
“Dipole dispersion”

These stable arrangements have minimal *long-range* stress fields.

Discrete Dislocation Dynamics

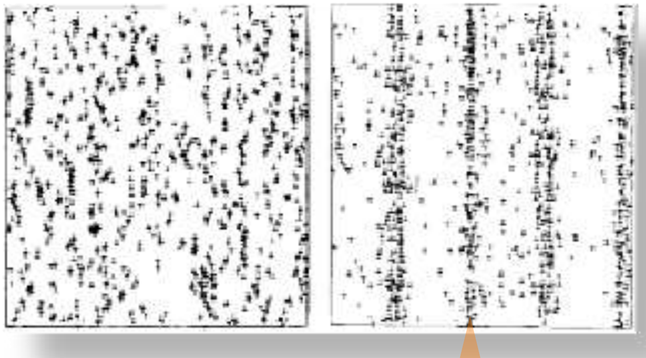
Discrete Dislocation Dynamics in 2D

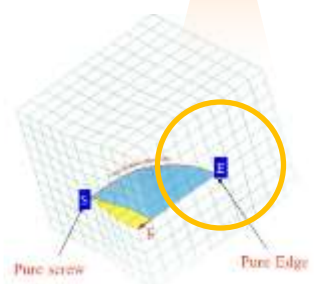
2D – view parallel to dislocation line



Discrete Dislocation Dynamics in 2D

2D – view parallel to dislocation line





Some questions:

Difference between edge and screw dislocations?

How to do multiplication?

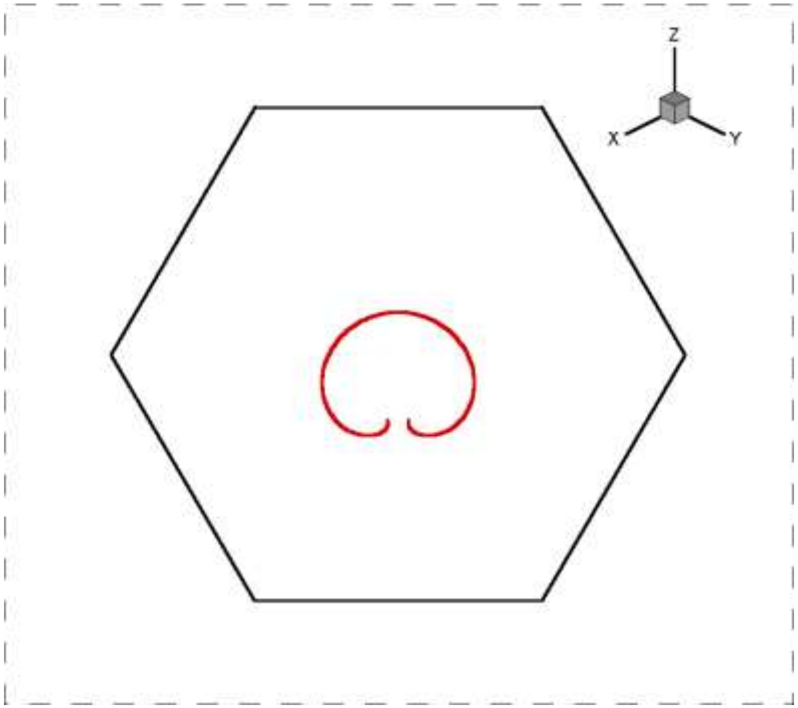
Dislocation bow-out?

Annihilation?

Climbing?

Discrete Dislocation Dynamics in 2D

2D – view into the glide plane



Discrete Dislocation Dynamics in 2D

2D – view into the glide plane

<u>Some questions:</u>

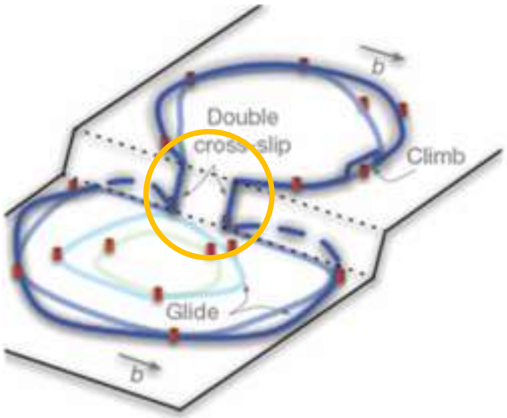
Difference between edge and screw dislocations?

Cross-slip?

Climb?

Cutting?

Jog-drag?



Discrete Dislocation Dynamics in 2D

2D – view into the glide plane

Some questions:

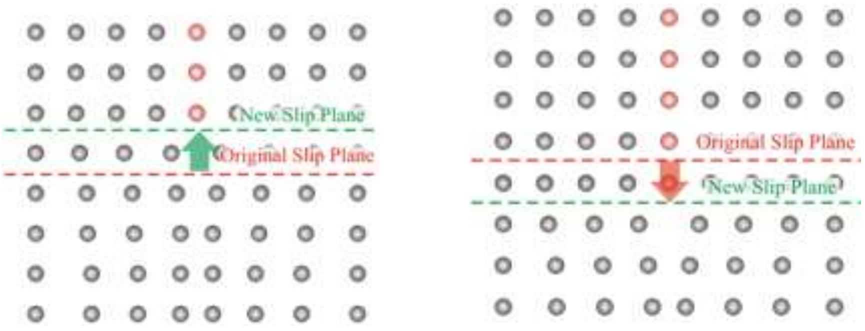
Difference between edge and screw dislocations?

Cross-slip?

Climb?

Cutting?

Jog-drag?



Discrete Dislocation Dynamics in 2D

2D – view into the glide plane

<u>Some questions:</u>

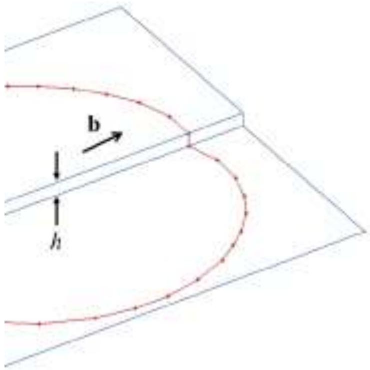
Difference between edge and screw dislocations?

Cross-slip?

Climb?

Cutting?

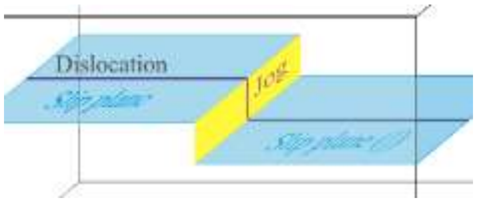
Jog-drag?



Dislocation-Dislocation Interactions

Straight dislocation can intersect to leave Jogs and Kinks in the dislocation line

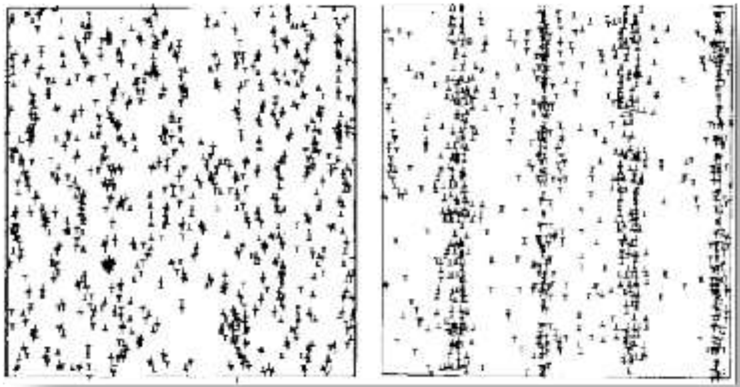
Extra segments in a dislocation line cost energy and require work done by the external force

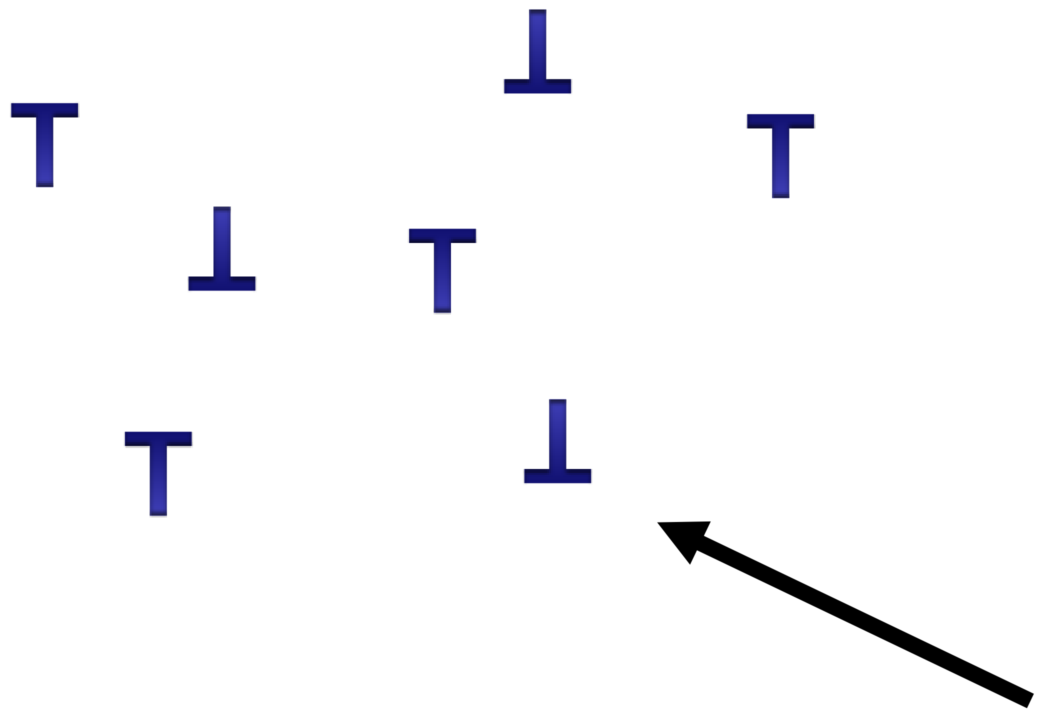


Discrete Dislocation Dynamics in 2D

2D – view parallel to dislocation line

Principle procedure





?

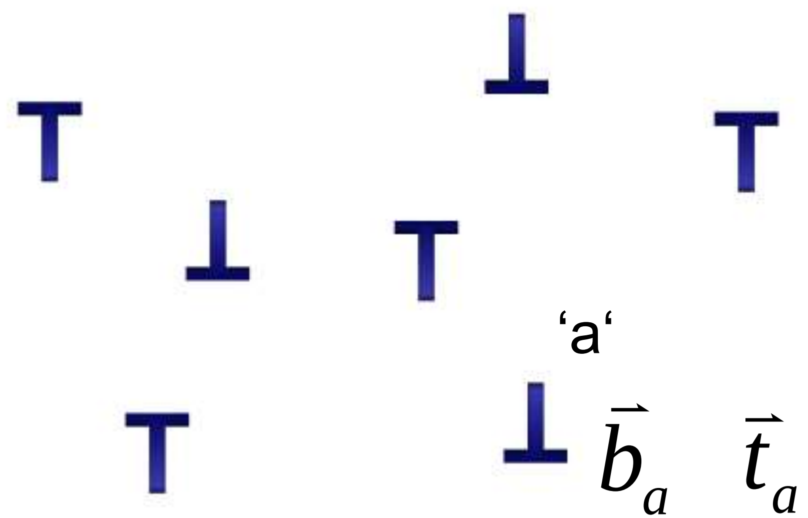
How to proceed?

Stress field of (edge) dislocation
Get coordinates
Use Peach Koehler
Move it

Basics of Discrete Dislocation Dynamics in 2D

Force $$\vec{F}_a = \left(\underline{\underline{\sigma}}^{\text{all others} \rightarrow a} \, \vec{b}_a \right) \times \vec{t}_a$$

Force on dislocation ‘a‘
by all others



Force $$\vec{F}_a = \left(\underline{\underline{\sigma}}^{\text{all others} \rightarrow a} \, \vec{b}_a \right) \times \vec{t}_a$$

Motion $$\underbrace{\vec{F} = \overbrace{m}^{\text{inertia}} \, \overbrace{\ddot{\vec{x}}}^{\text{acceleration}} + B\underbrace{\dot{\vec{x}}}_{\text{velocity}} \approx \overbrace{B}^{\text{friction coefficient (drag)}}\dot{\vec{x}}}$$

Equilibrium of forces

$$\sum \vec{F}_i = 0$$

$$\sum \vec{F}_i = B\dot{\vec{x}} + \vec{F}_a = 0$$

$$\vec{F}_a = \left(\underline{\underline{\sigma}}^{\text{alle}\to a} \; \vec{b}_a \right) \times \vec{t}_a$$

Equilibrium of forces

$$\boxed{\sum F = 0}$$

$$\boxed{F_{disloc} + F_{self\ force} + F_{extern} + F_{therm} + F_{viscous} + F_{obstacle} + F_{Peierls} + F_{osmotic} + F_{image} + F_{inertia}}$$

F_{disloc} : elastic – other dislocations

$F_{self\ force}$: elastic – self

F_{extern} : external

F_{therm} : Stochastic Langevin

$F_{viscous}$: viscous drag

$F_{obstacle}$: obstacle

$F_{Peierls}$: Peierls

$F_{osmotic}$: chemical forces

F_{image} : surface forces

$F_{point\ defect}$: point defects

Example of Discrete Dislocation Dynamics in 2D

1

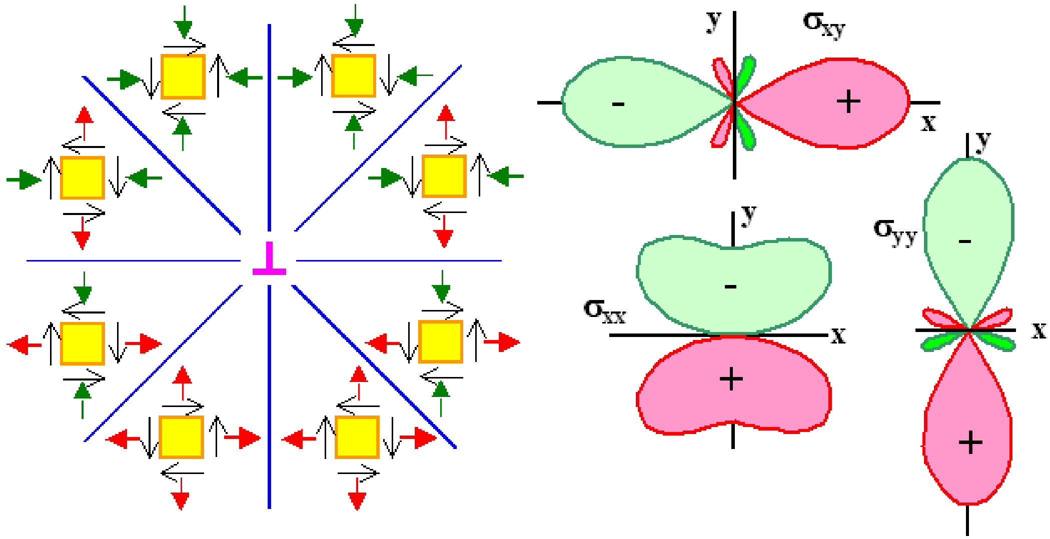
$$\sigma_{xz} = \sigma_{zx} = \sigma_{yz} = \sigma_{zy} = 0$$

$$\sigma_{xx} = -D\,y \frac{3x^2 + y^2}{\left(x^2 + y^2\right)^2}, \qquad \text{with:} \quad D = \frac{Gb}{2\pi(1-\nu)}$$

$$\sigma_{yy} = D\,y \frac{x^2 - y^2}{\left(x^2 + y^2\right)^2}$$

$$\sigma_{xy} = \sigma_{yx} = D\,x \frac{x^2 - y^2}{\left(x^2 + y^2\right)^2}$$

$$\sigma_{zz} = \nu\left(\sigma_{xx} + \sigma_{yy}\right)$$



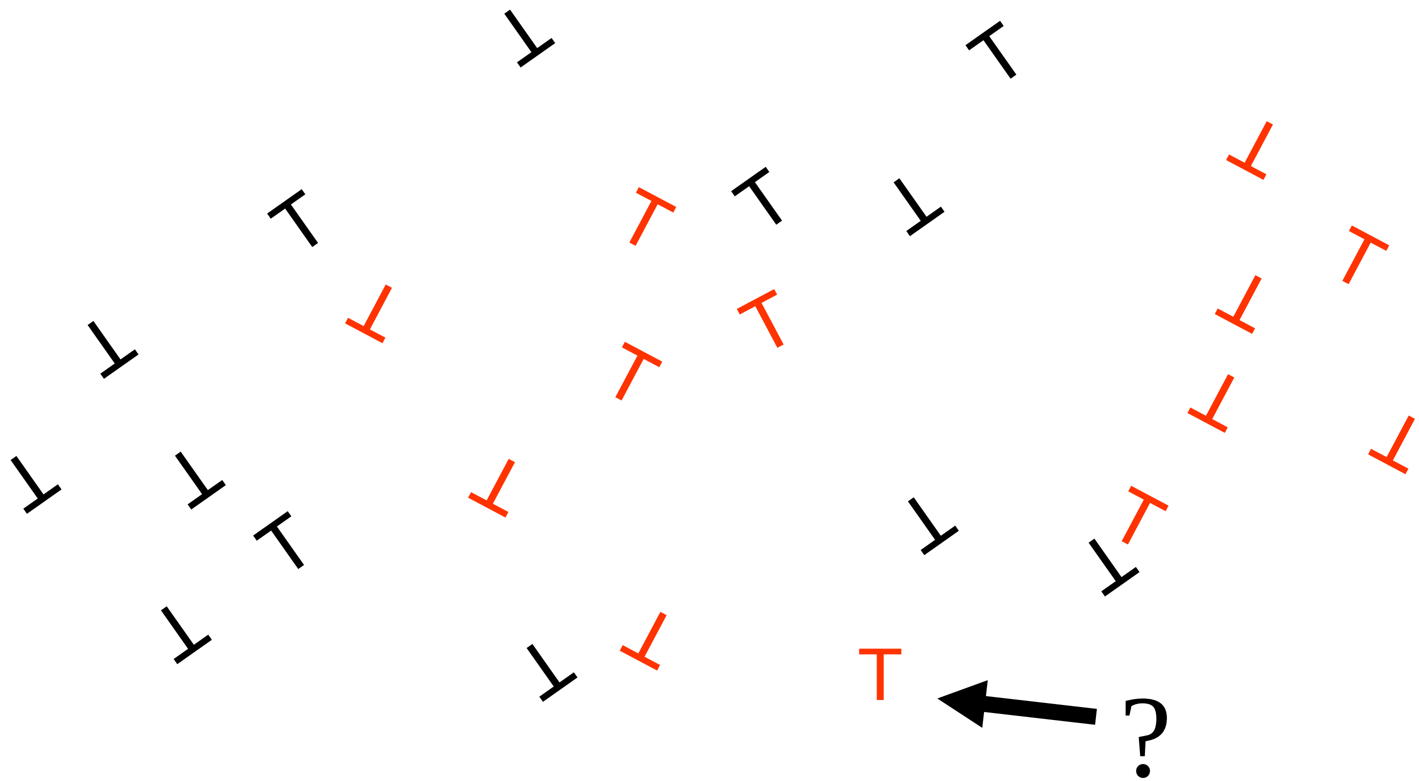
2

$$\vec{F}_a = \left(\underline{\underline{\sigma}}^{\text{all}\rightarrow a}\ \vec{b}_a \right) \times \vec{t}_a$$

3

$$\vec{F}_a + B\dot{\vec{x}} + \vec{F}_{external} = 0$$

Example of Discrete Dislocation Dynamics in 2D



Example of Discrete Dislocation Dynamics in 2D

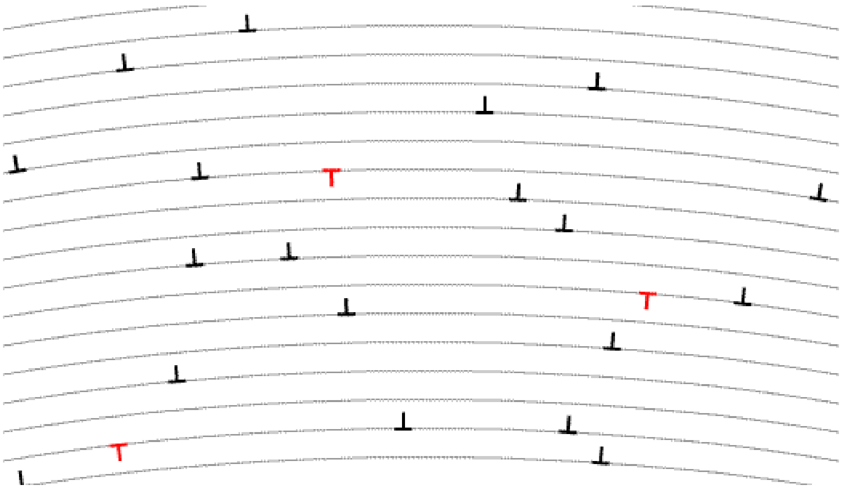
T ← ?

1) Calculate stress field of machine and of all other dislocations at position of T

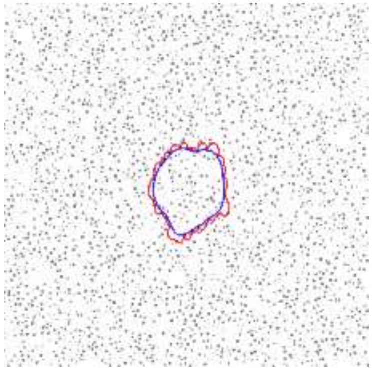
2) Use Peach-Koehler equation to get force on dislocation

3) Integrate with very small time step (explicit) viscous eq. of motion

Example of Discrete Dislocation Dynamics in 2D

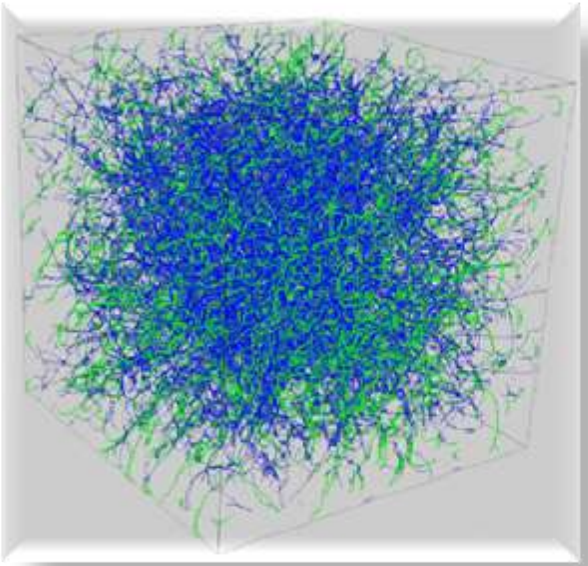


Example of Discrete Dislocation Dynamics in 2D



Discrete Dislocation Dynamics in 3D

Full 3D segment treatment



Some questions:

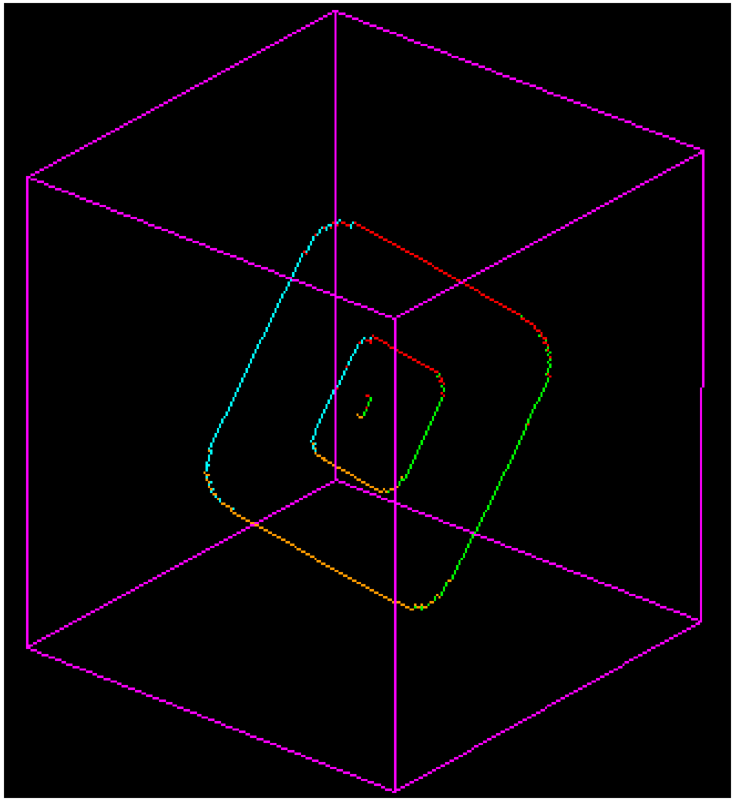
Difference between edge and screw dislocations?

Junctions?

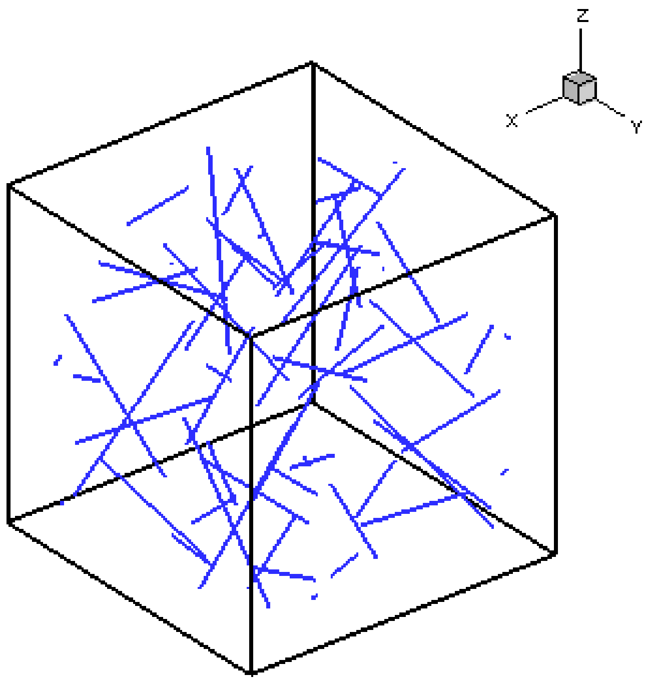
Cutting?

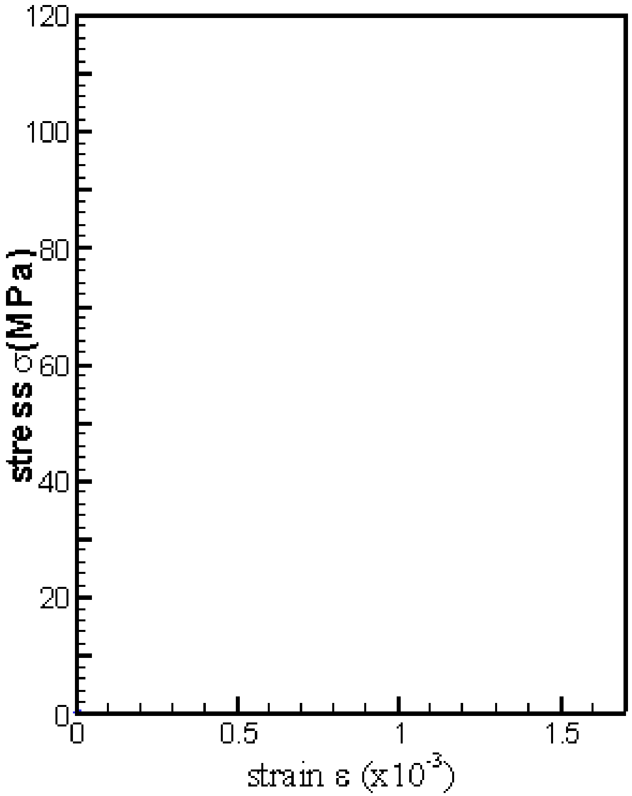
Cores of the dislocations?

Example of Discrete Dislocation Dynamics in 3D

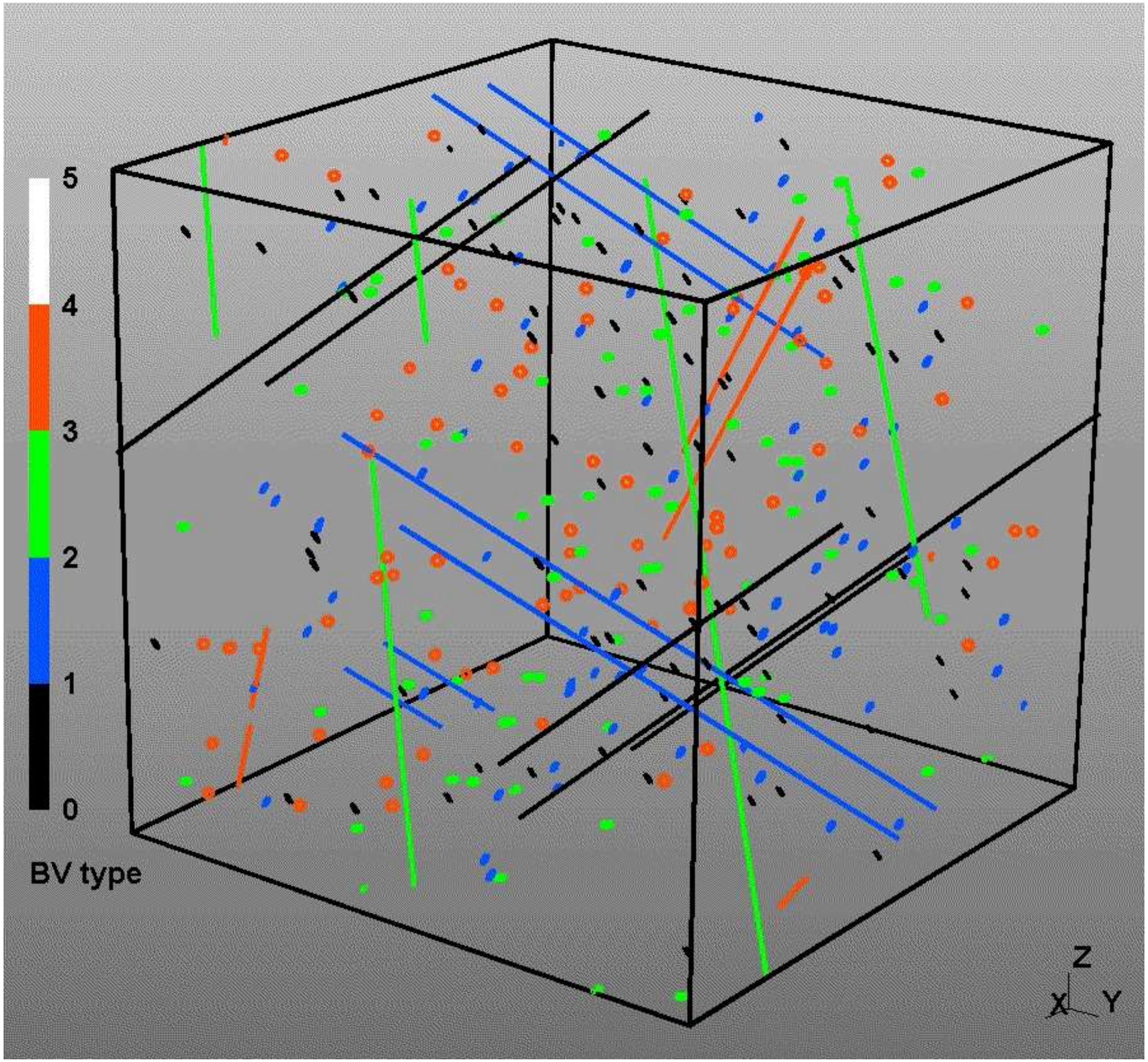


3D: DDD (discrete dislocation dynamics)

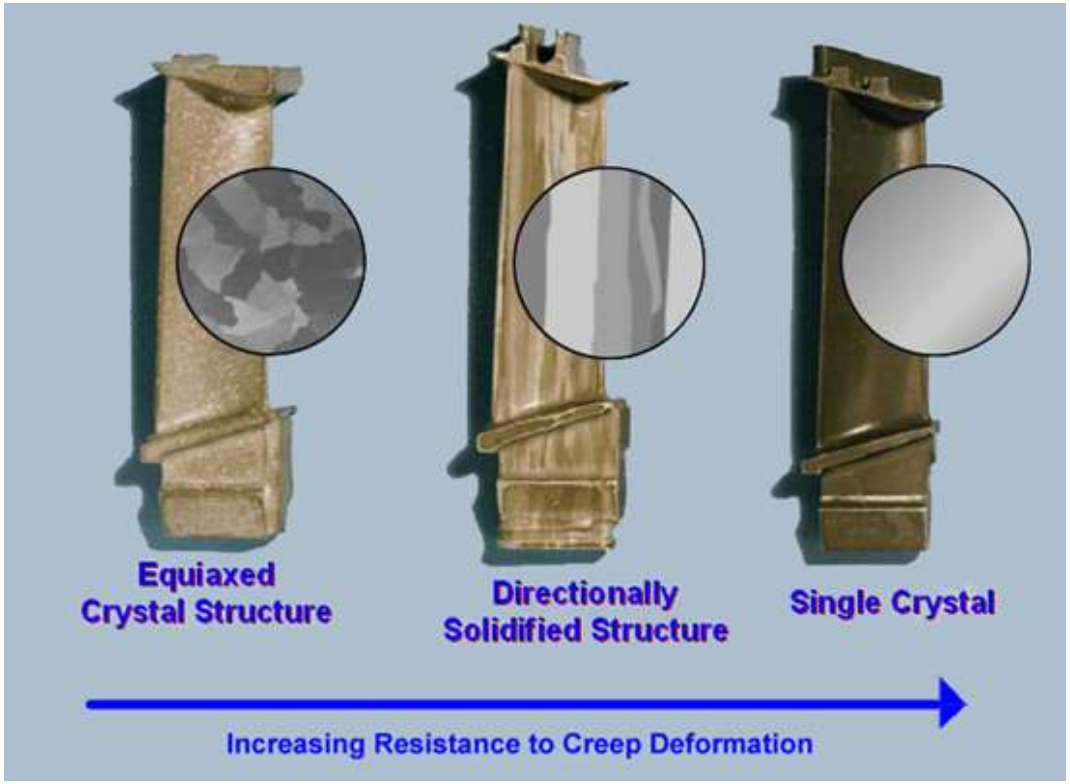




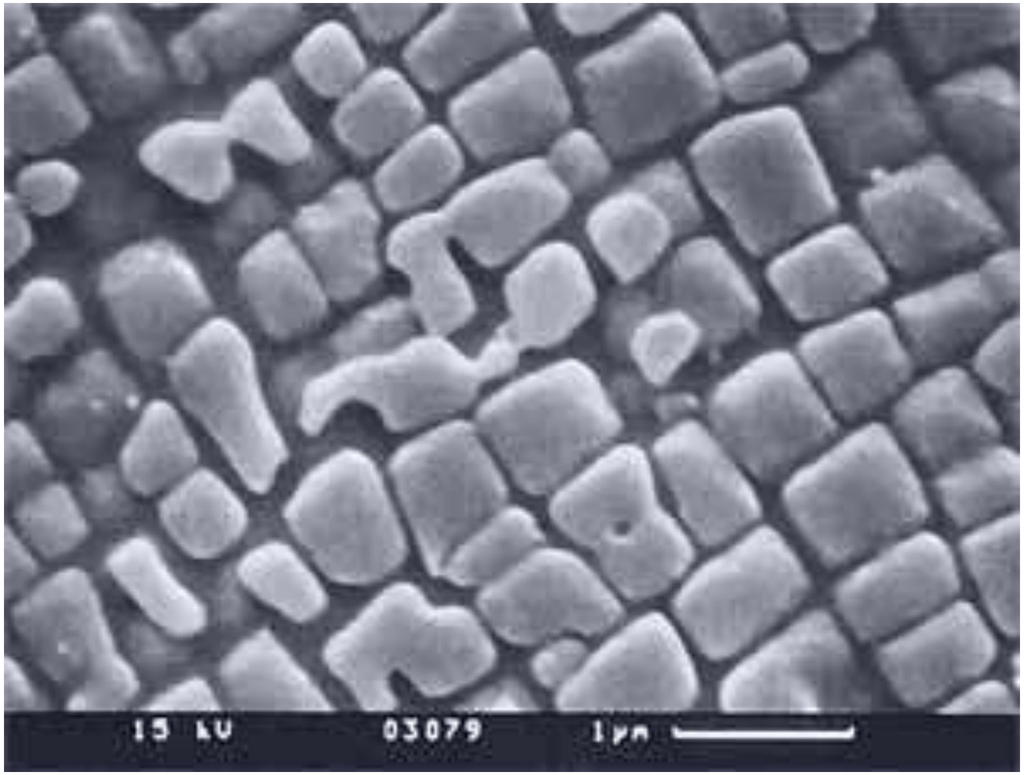
Example of Discrete Dislocation Dynamics in 3D



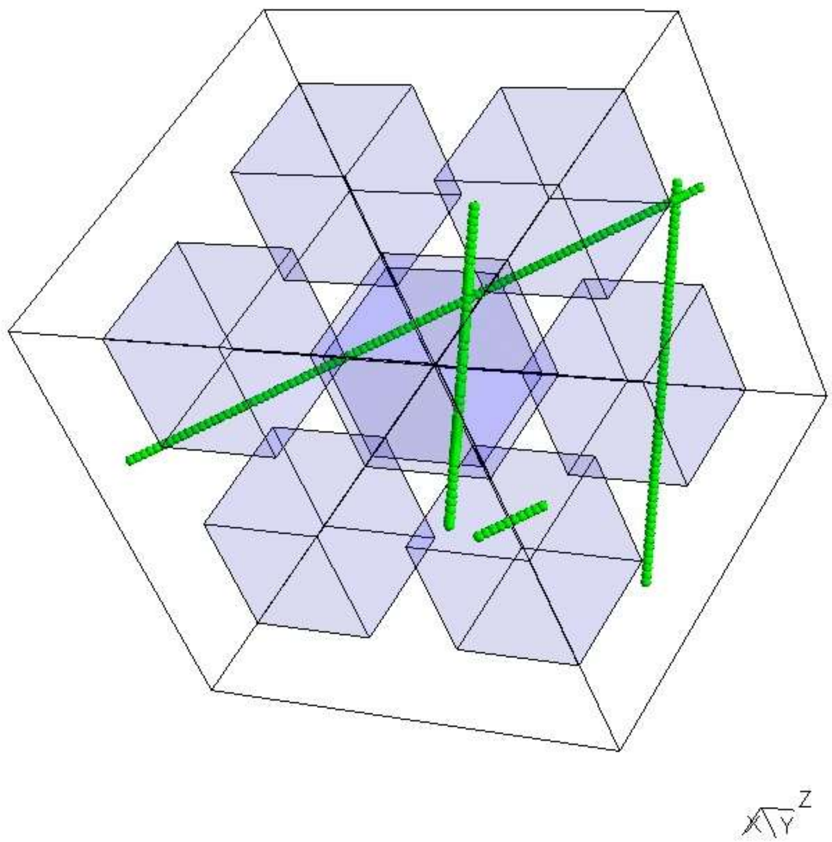

Write down the
(v) Calculate
and
constants a, b and c.
for i = 1, . . . , n
f(x) =
ck of memory', propert
terms of

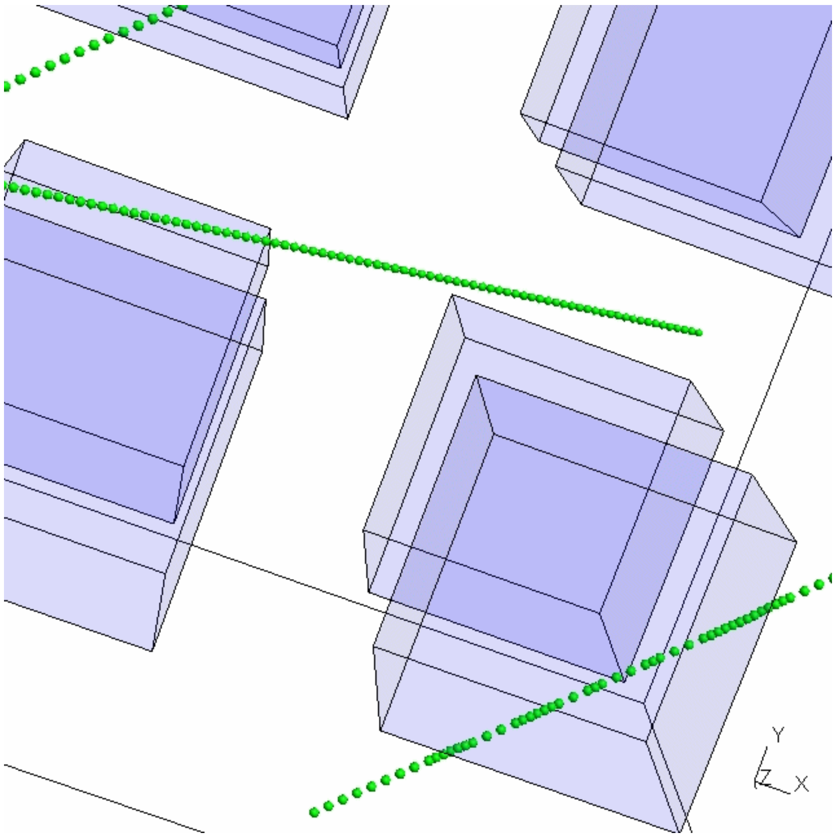

Equiaxed
Crystal Structure
Directionally
Solidified Structure
Single Crystal
Increasing Resistance to Creep Deformation

Example of Discrete Dislocation Dynamics in 3D: superalloys

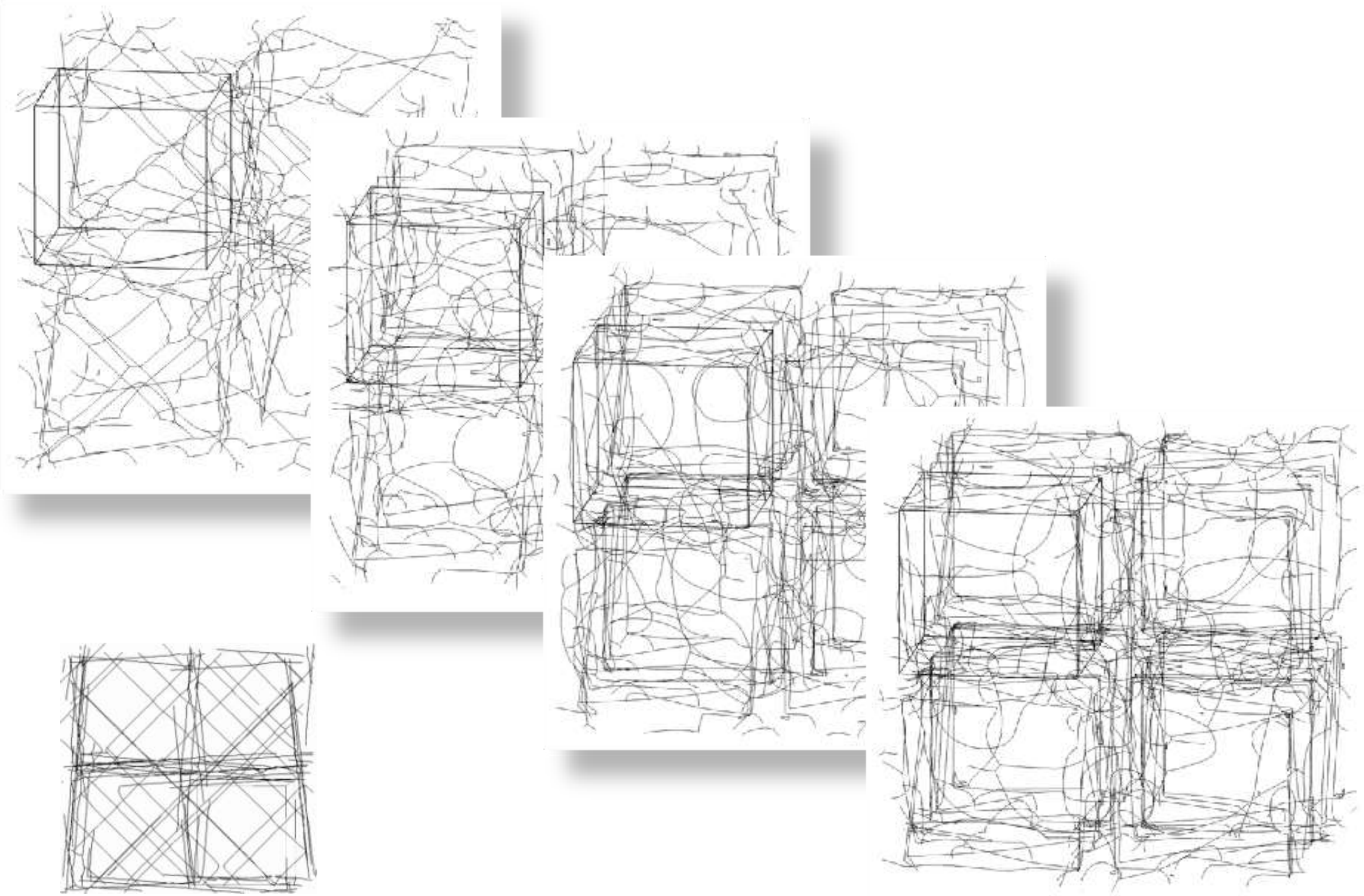


Example of Discrete Dislocation Dynamics in 3D

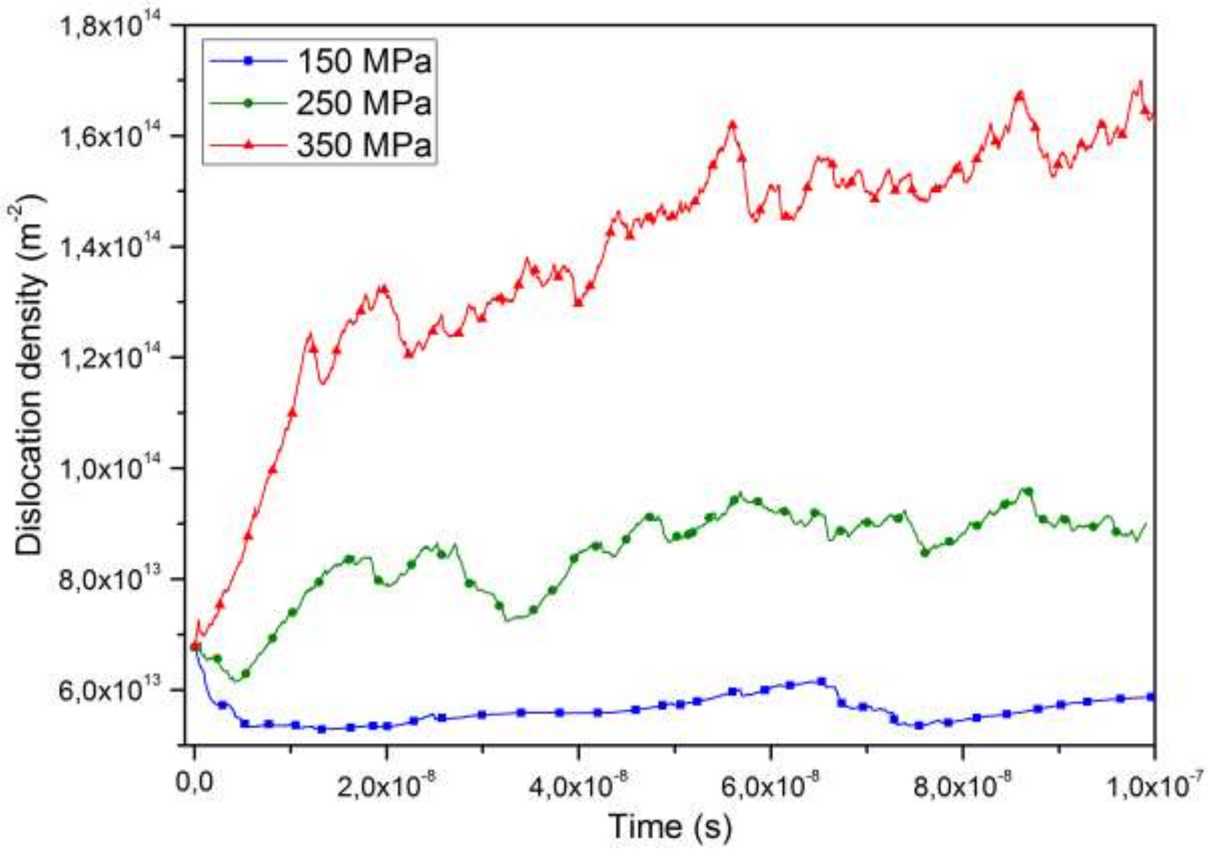




Example of Discrete Dislocation Dynamics in 3D: superalloys



Example of Discrete Dislocation Dynamics in 3D: superalloys



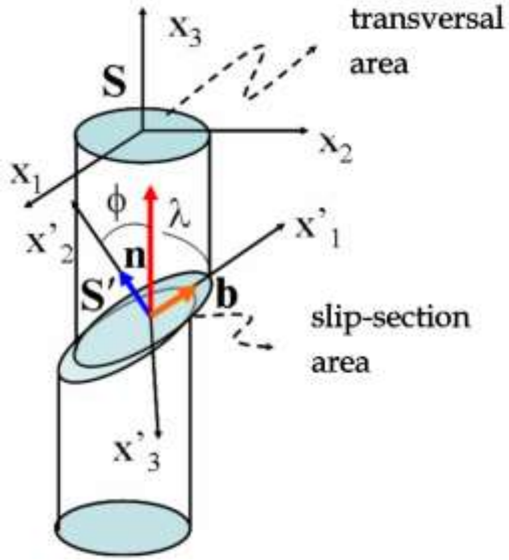
Overview

- **Some basic methods**
  - Atomistic
  - Monte Carlo
  - Dislocations
  - Polycrystal mechanics

- **Ab-initio informed constitutive models**
  - Elasticity: from DFT to Homogenization
  - Atomistically informed simulation: from APT to MD
  - From DFT to dislocation rate models and yield surfaces

DFT: Density Functional Theory; APT: Atom Probe Tomography; MD: Molecular Dynamics; RVE: Representative Volume Element; ICME: Integrated Computational Materials Engineering

Single crystal plasticity: constructing the yield surface

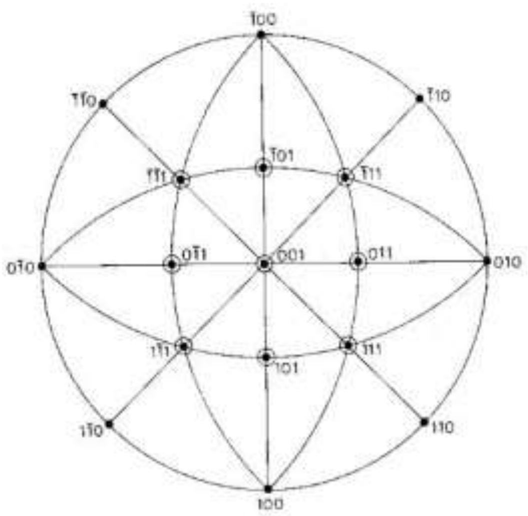


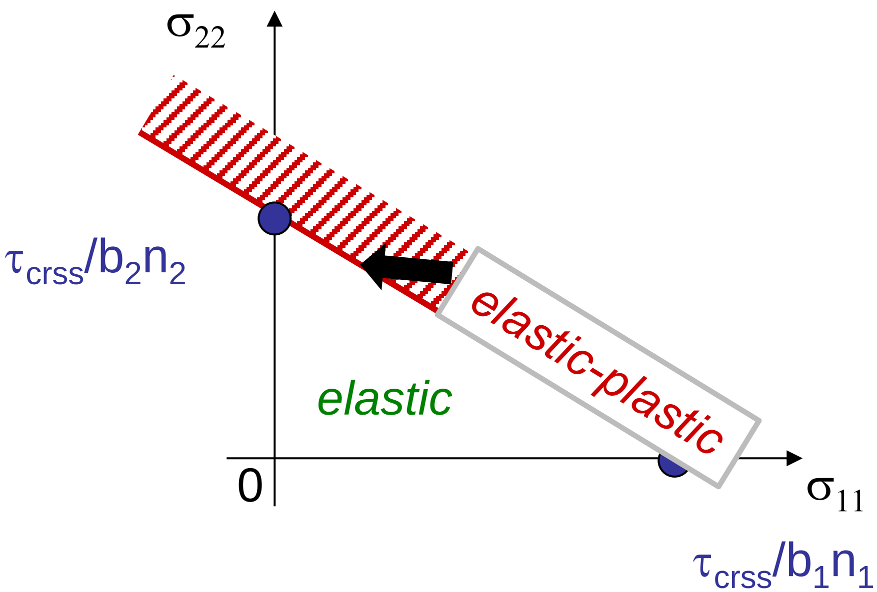
- Yield criterion for single slip:

$$\sigma_{ij}\, b_i\, n_j = \tau_{crss}$$

- In 2D this becomes ($\sigma_1 \equiv \sigma_{11}$:

$$\sigma_{11}\, b_1\, n_1 + \sigma_{22}\, b_2\, n_2 = \tau_{crss}$$





Single crystal plasticity: constructing the yield surface

What is the straining direction?

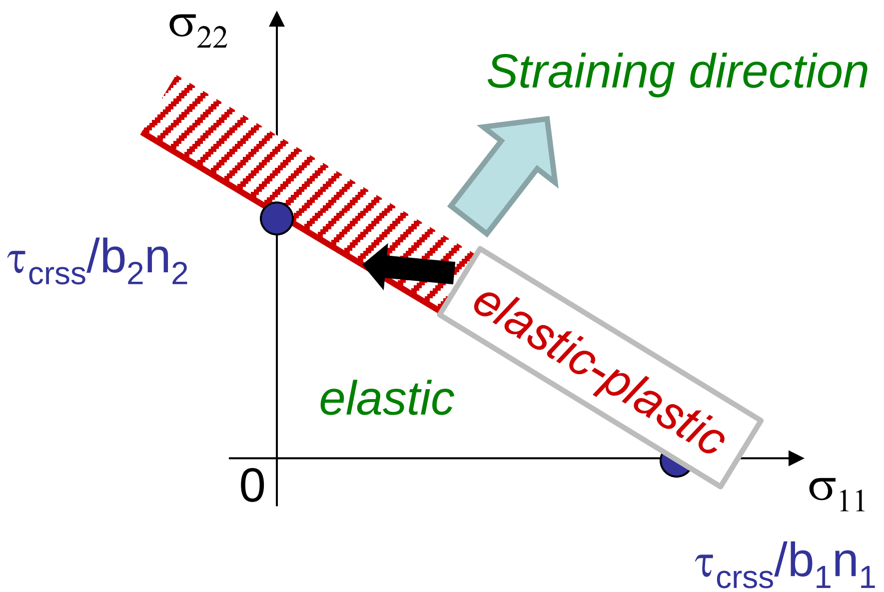
The strain increment is given by:

$$d\varepsilon = \Sigma_s \, d\gamma^{(s)} b^{(s)} n^{(s)}$$

2D case:

$$d\varepsilon_1 = d\gamma \, b_1 n_1; \; d\varepsilon_2 = d\gamma \, b_2 n_2$$

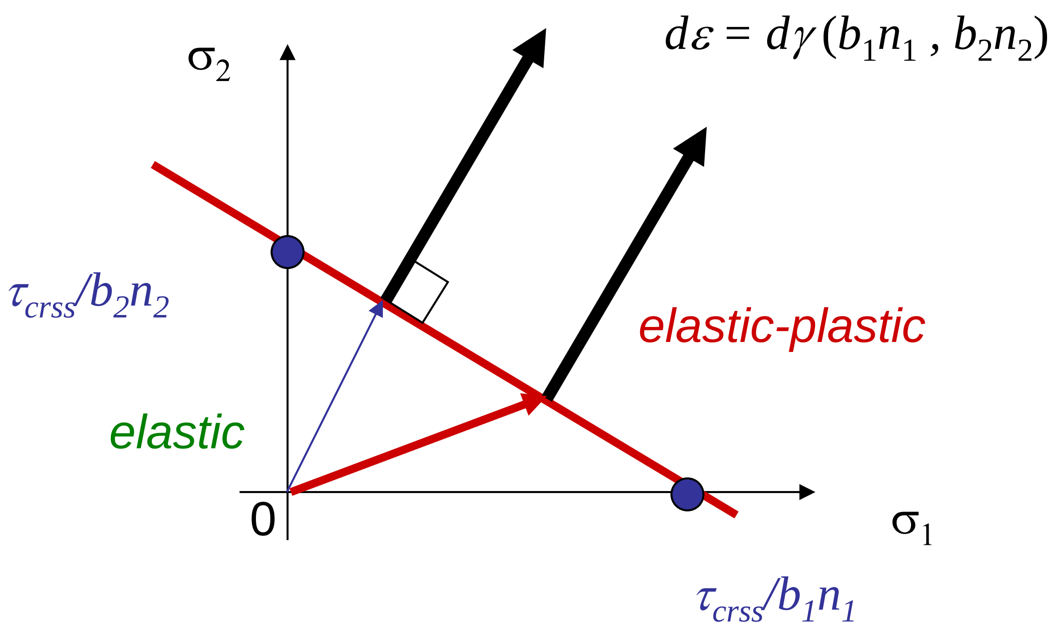
vector perpendicular to the line for yield



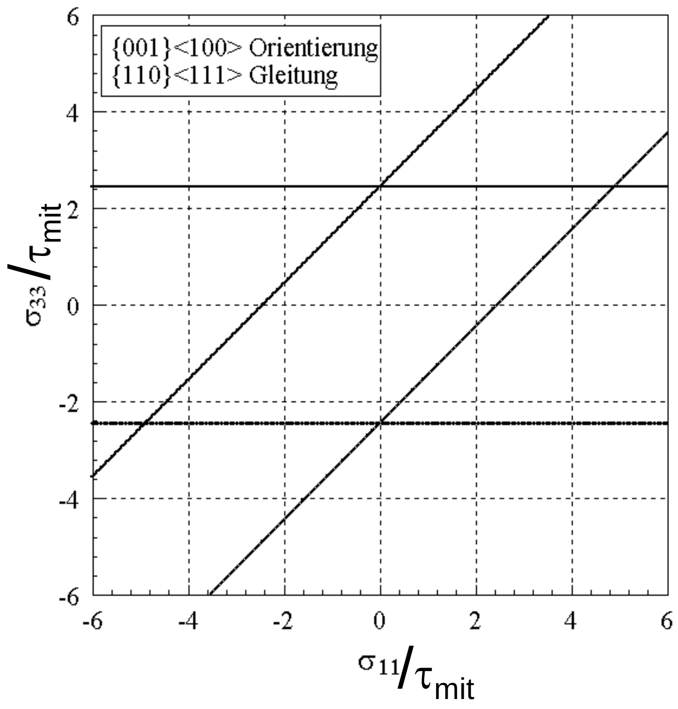
straining direction in stress space

normality rule for crystallographic slip

Any given stress state can in a crystal in large-strain elasto-plasticity act only in the form of shear (except hydrostatic effects)



Single crystal plasticity: constructing the yield surface



slip system s

$n_i^s\,,\, b_i^s$

orientation factor for s

$m_{ij}^s = n_i^s\, b_j^s$

symmetric part $$m_{ij}^{sym,s} = \frac{1}{2}\left(n_i^s\, b_j^s + n_j^s\, b_i^s\right)$$

rotate crystal into sample $$m_{kl}^s = a_{ki}^c\, n_i^s\; a_{lj}^c\, b_j^s$$

symmetric part $$m_{kl}^{sym,s} = \frac{1}{2}\left(a_{ki}^c\, n_i^s\; a_{lj}^c\, b_j^s + a_{lj}^c\, n_j^s\; a_{ki}^c\, b_i^s\right)$$

yield surface
(active systems)

$$\boxed{\begin{aligned} m_{kl}^{sym,s=aktiv}\,\sigma_{kl} &= \sigma_{aufg}^s = \tau_{krit,(+)}^{s=aktiv} \\ m_{kl}^{sym,s=aktiv}\,\sigma_{kl} &= \sigma_{aufg}^s = \tau_{krit,(-)}^{s=aktiv} \end{aligned}}$$

(non-active systems) $$m_{kl}^{sym,s=inaktiv}\,\sigma_{kl} = \sigma_{aufg}^s < \tau_{krit,(\pm)}^{s=inaktiv}$$

Active slip system:

$$\tau^{\alpha} = \tau_{\text{crit}}$$

$$\tau^{\alpha} \approx \boldsymbol{T}_{\text{e}} \cdot \boldsymbol{S}_{0}{}^{\alpha}$$

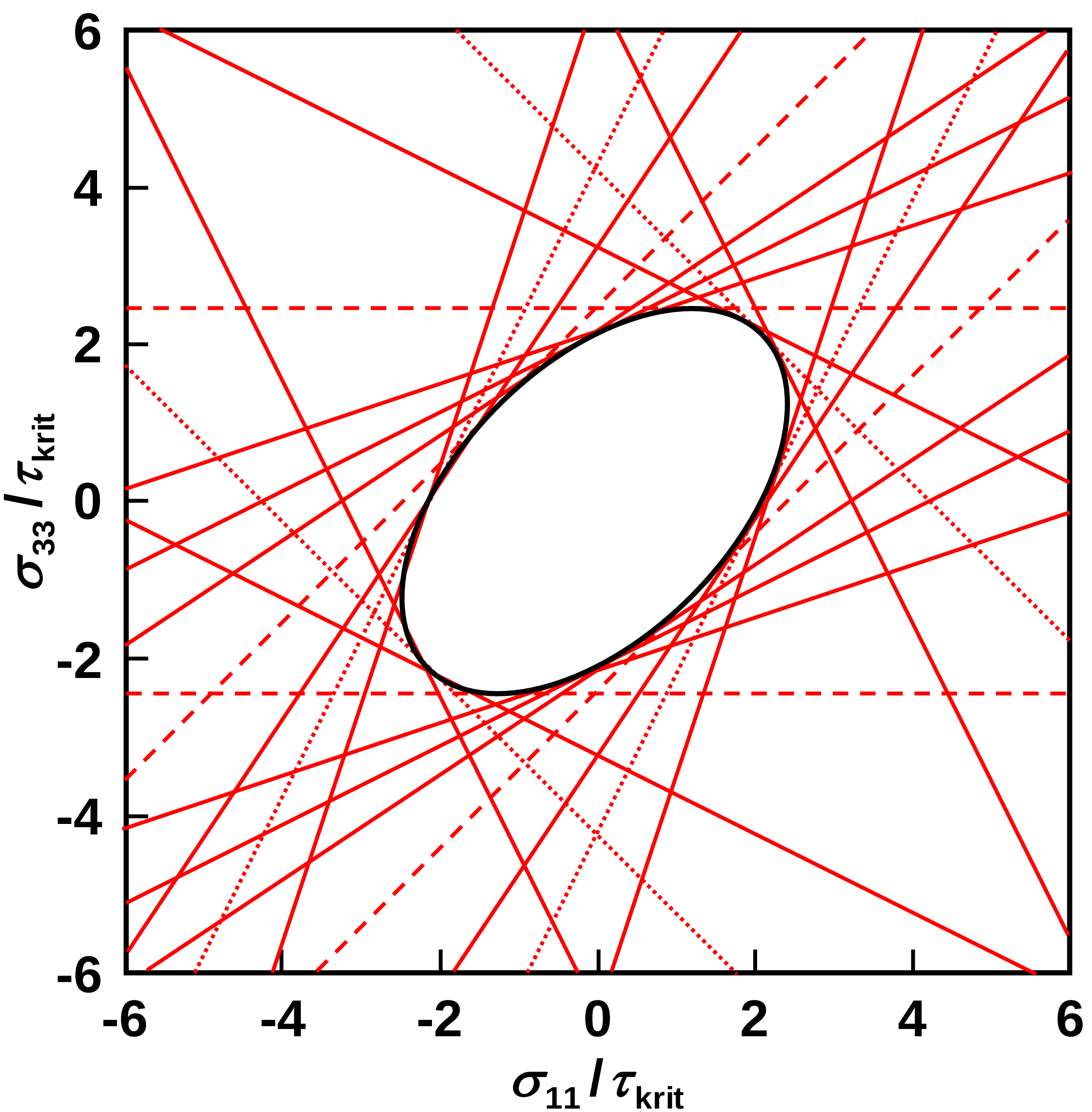
with $\boldsymbol{S}_{0}{}^{\alpha} = \boldsymbol{m}_{0}{}^{\alpha} \otimes \boldsymbol{n}_{0}{}^{\alpha}$

bcc 48 slip systems
orientation {001}<100>

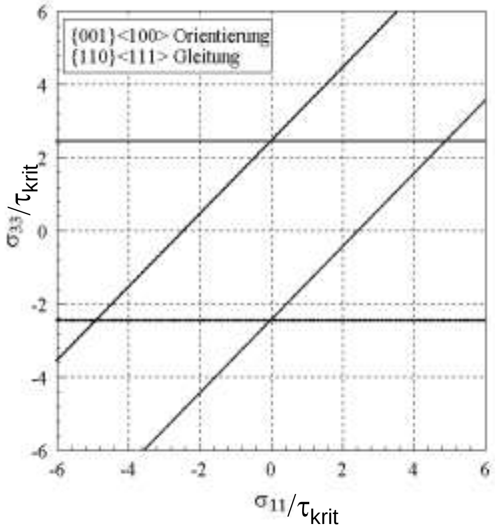
12 x {110}<111> – – –

12 x {112}<111> ··········

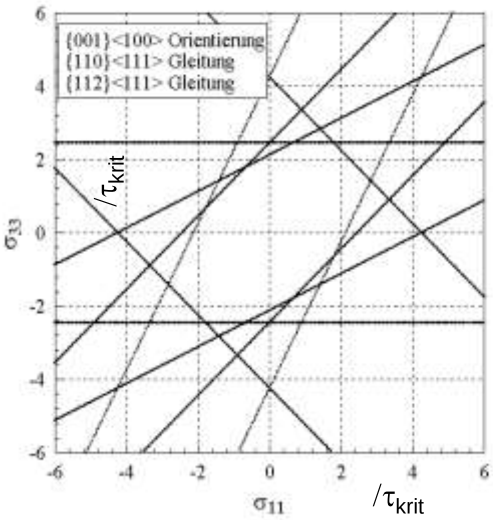
24 x {123}<111> ——



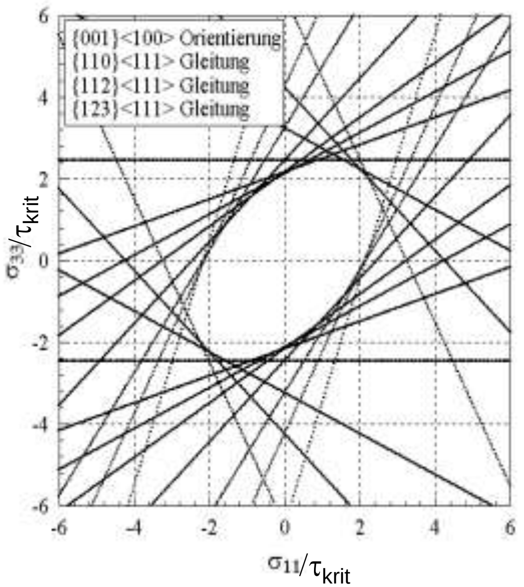
Single crystal plasticity: constructing the yield surface



FCC, BCC
12 systems
section



BCC
24 systems
section



BCC
48 systems
section

yield surface, bcc

single crystal, bcc, (001)[100]

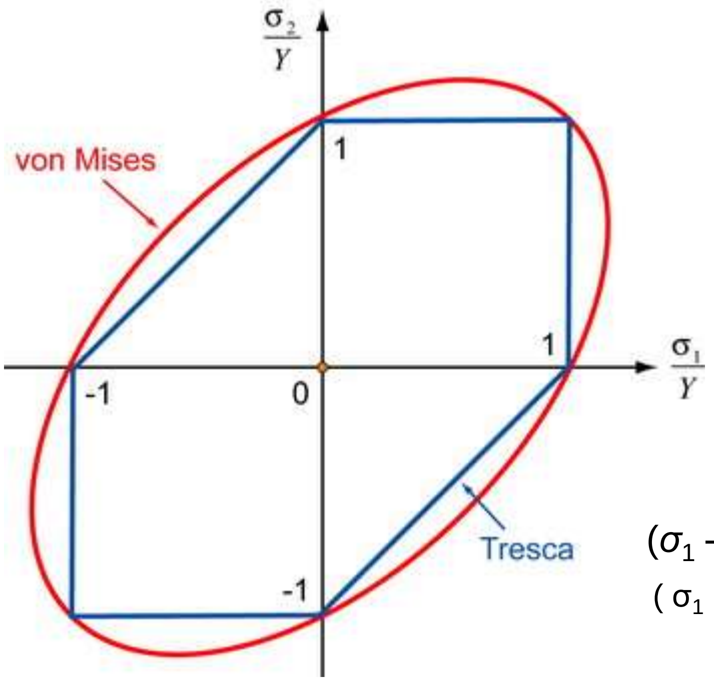
Macroscopic – empiricial yield criteria

Yield criterion: determine the critical stress required to cause permanent deformation

Many different macroscopic yield criteria

σ_{ij} stress acting on a solid
σ1, σ2, σ3 principal values of stress tensor
Y yield stress of the material in uniaxial tension

$$(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 = \text{constant}$$



$$(\sigma_1 - \sigma_3) = Y$$

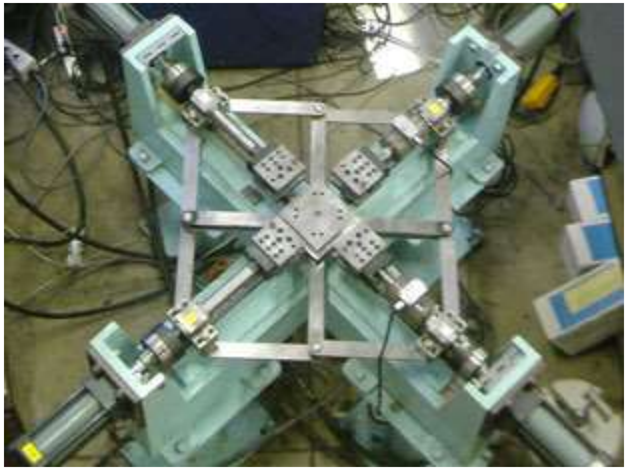
$$(\sigma_1 > \sigma_2 > \sigma_3)$$

Macroscopic yield criteria

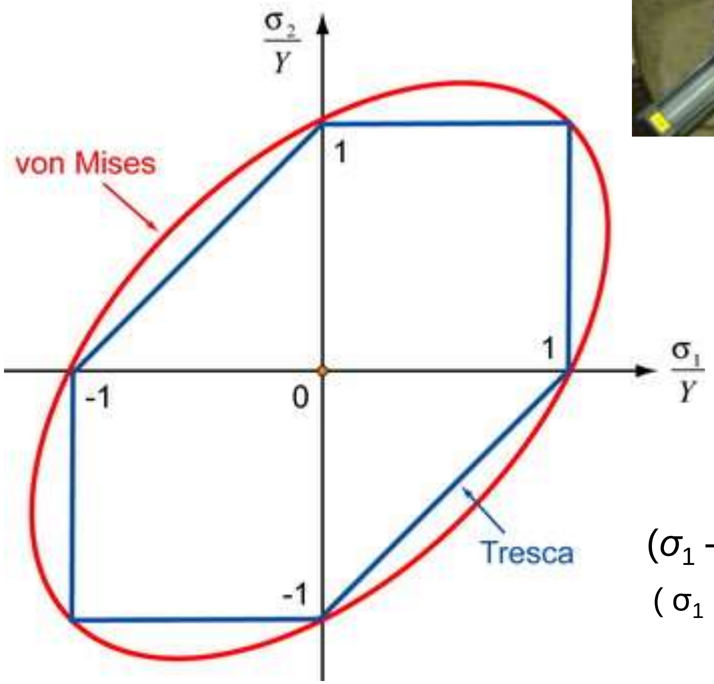
Yield criterion: determine the critical stress required to cause permanent deformation

Many different macroscopic yield criteria

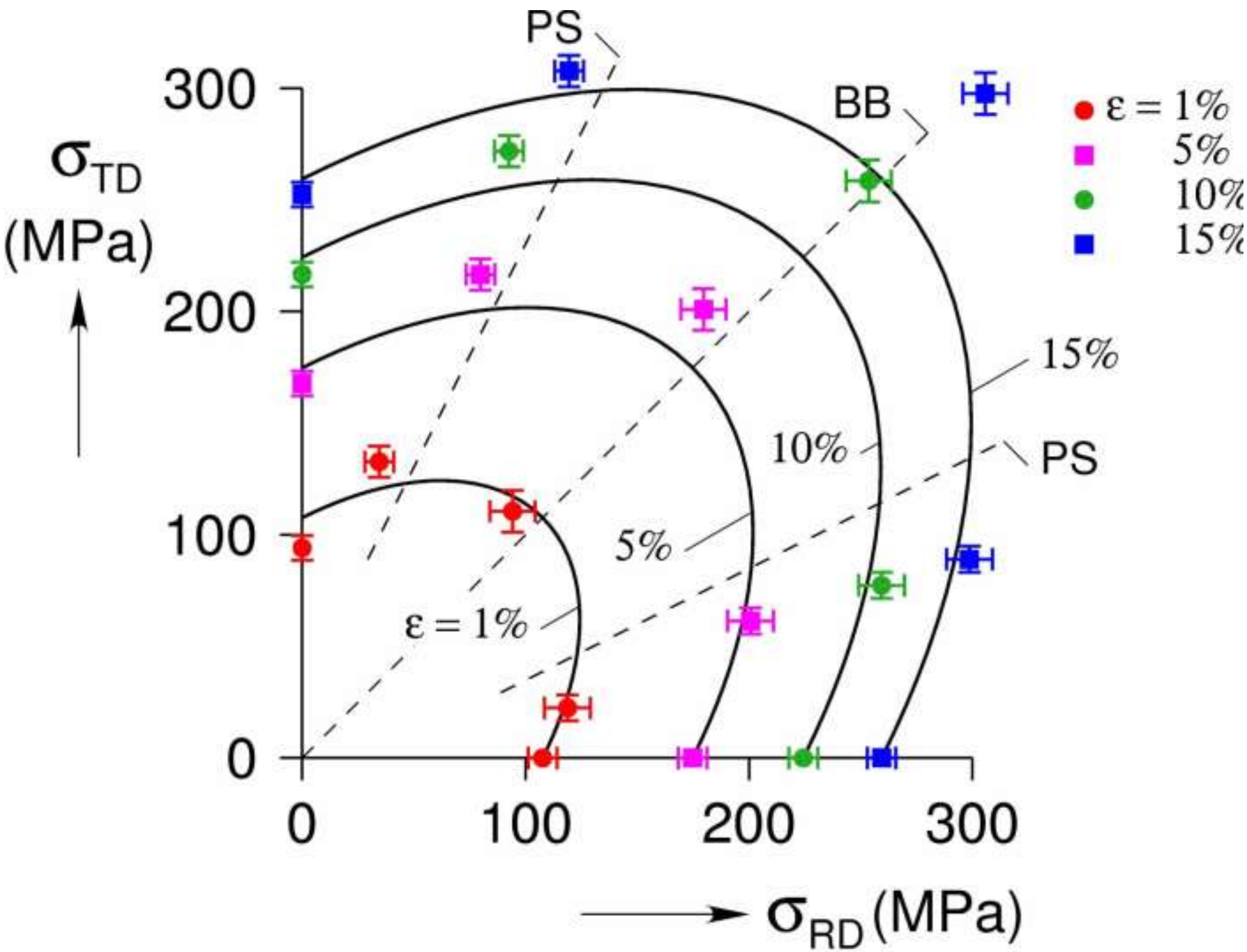
σ_{ij} stress acting on a solid
$\sigma1$, $\sigma2$, $\sigma3$ principal values of stress tensor
Y yield stress of the material in uniaxial tension



$$(\sigma_1-\sigma_2)^2+(\sigma_2-\sigma_3)^2+(\sigma_3-\sigma_1)^2=\text{constant}$$

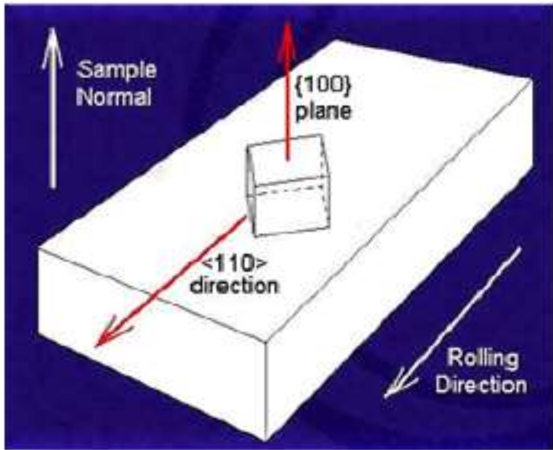


$$(\sigma_1-\sigma_3)=Y$$
$$(\sigma_1>\sigma_2>\sigma_3)$$

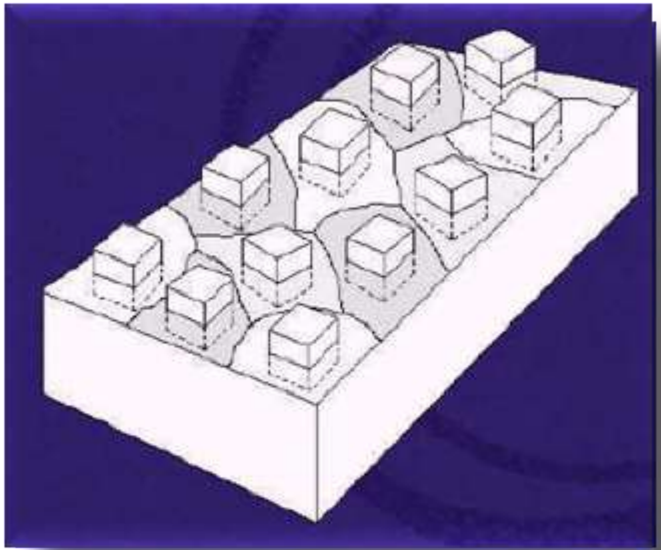


PS
300
BB
σ_{TD} (MPa)
200
100
0
0
100
200
300
15%
10%
5%
$\varepsilon = 1\%$
PS
σ_{RD} (MPa)
$\varepsilon = 1\%$
5%
10%
15%

Crystal rotations under heterogeneous constraints



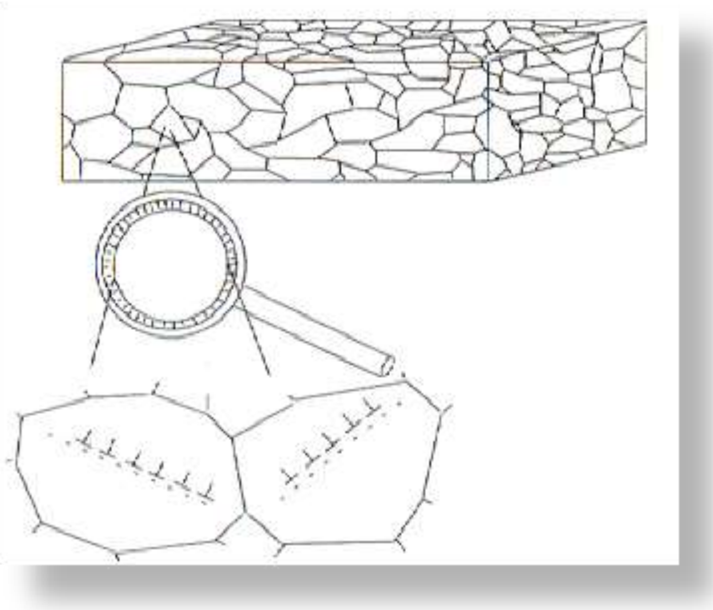
Grains in polycrystals do NOT experience the same boundary conditions.

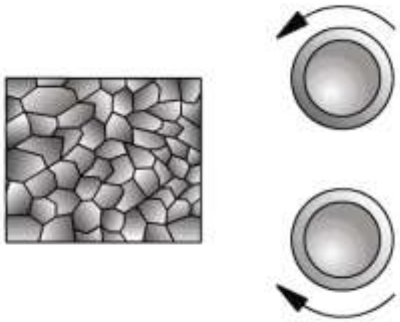


Differentiate between GLOBAL bounday conditions (tool, process) and the LOCAL (micromechanical) boundary conditions. The latter are influenced by grain-to-grain interactions and local inhomogeneity.

Raabe et al. Acta Mat. 49 (2001)

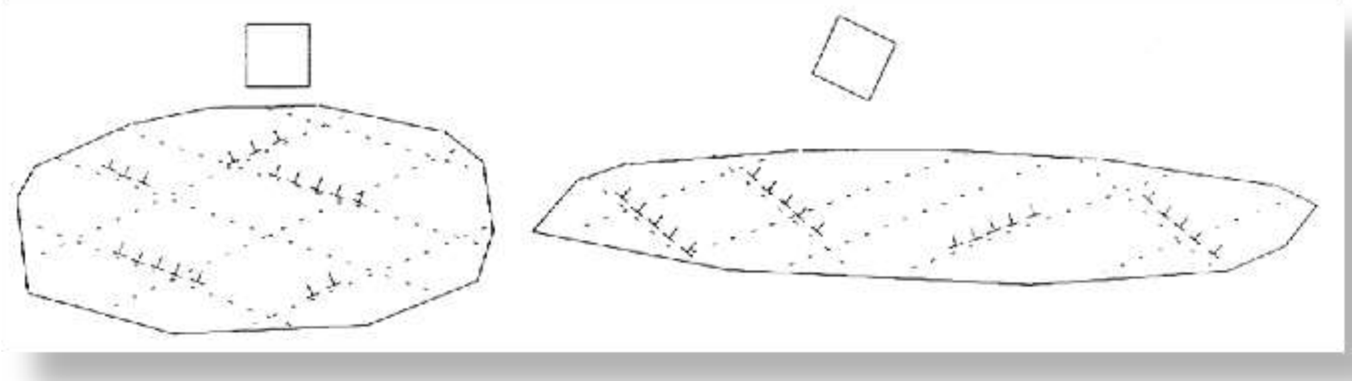
The Taylor Model





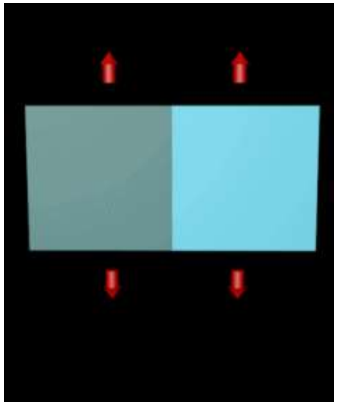
$$\varepsilon_{ij} = \frac{1}{2} \sum_{s=1}^{5} \left(n_i^s b_j^s + n_j^s b_i^s \right) \gamma^s$$

$$\varepsilon_{ij}=\frac{1}{2}\sum_{s=1}^{5}\left(n_i^s b_j^s+n_j^s b_i^s\right)\gamma^s$$

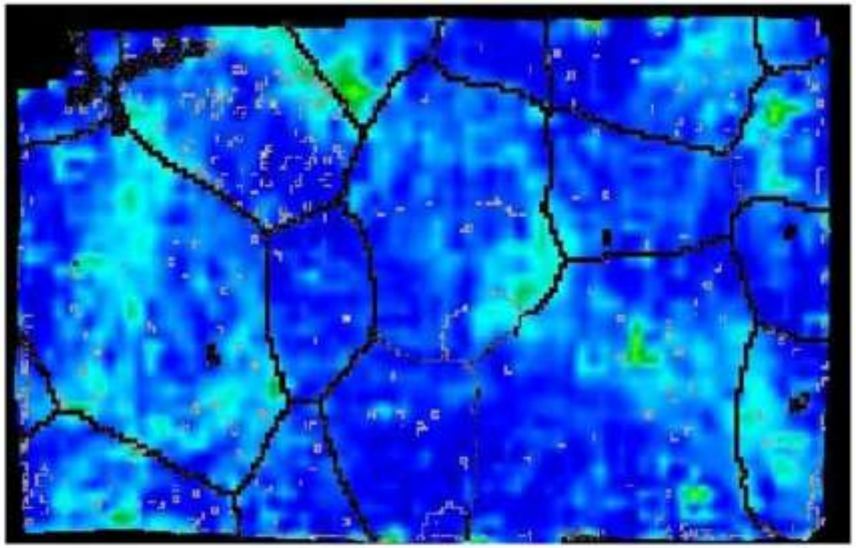


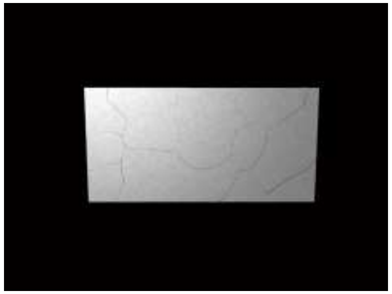
plastic spin from polar decomposition

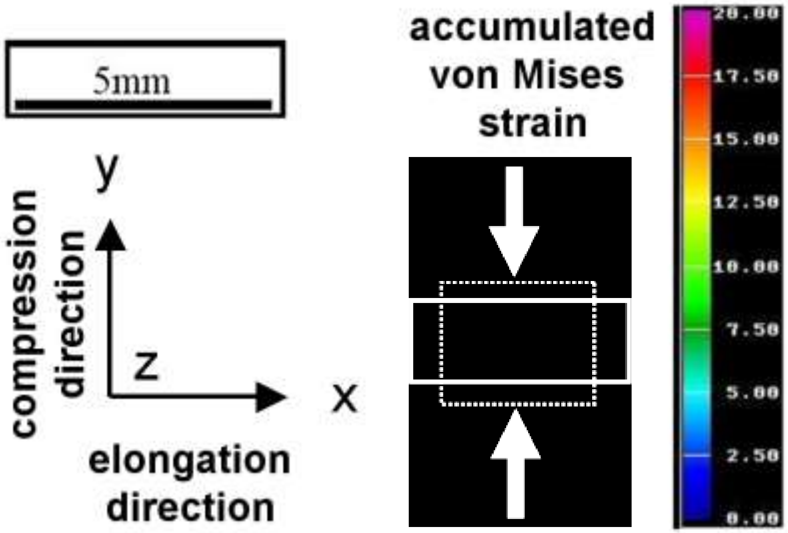
$$\dot{\omega}_{ij}^{K}=W_{ij}^{K}=\frac{1}{2}\left(\dot{u}_{i,j}^{\mathrm{K}}-\dot{u}_{j,i}^{\mathrm{K}}\right)=\sum_{s=1}^{N} m_{ij}^{\mathrm{asym},s}\,\dot{\gamma}^{s}$$



3%



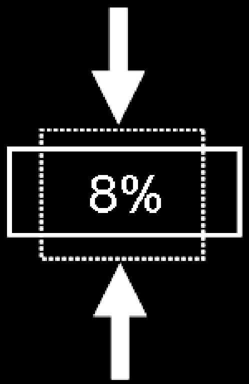


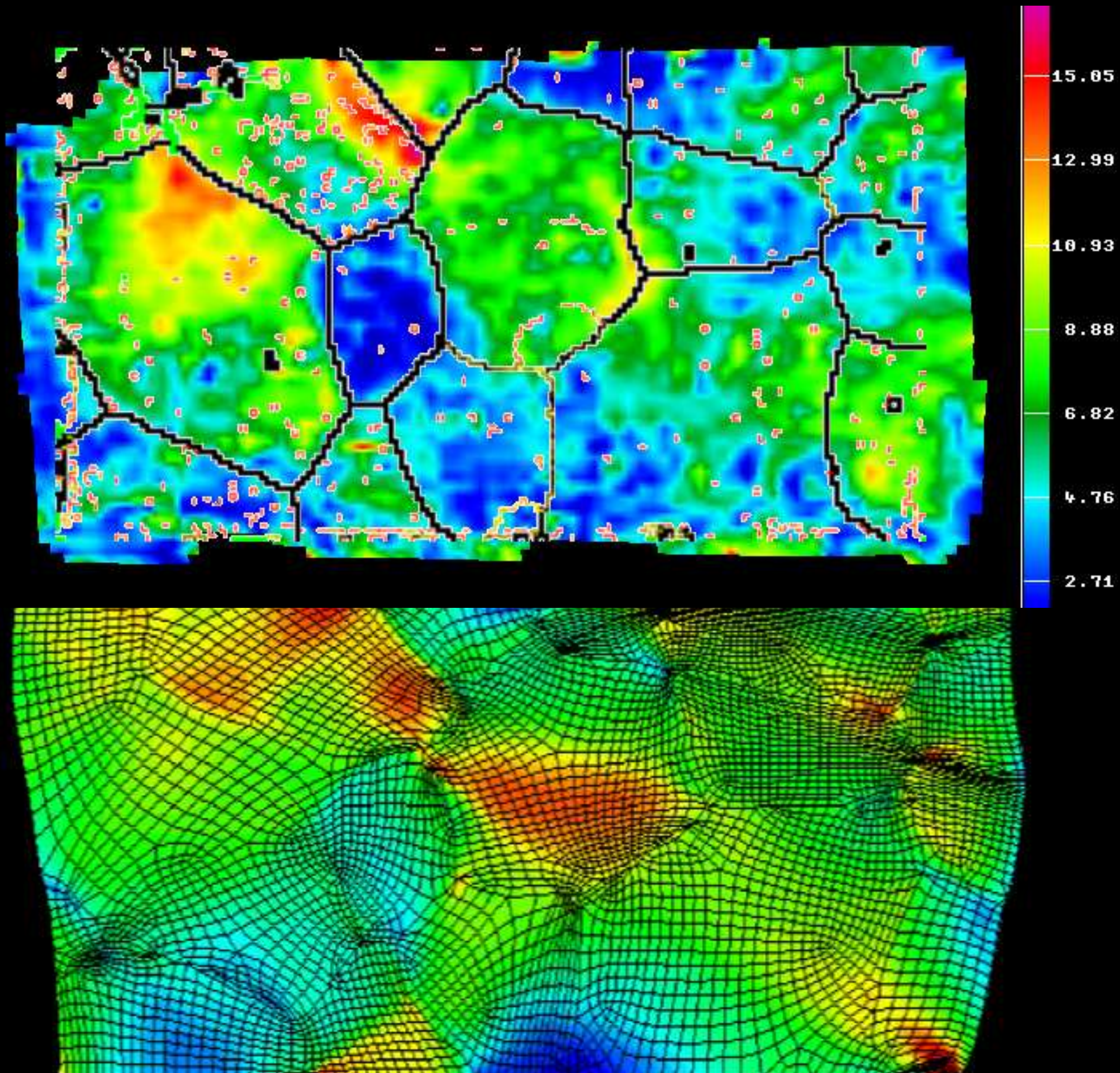


Raabe et al. Acta Mater. 49 (2001) 3433

Sachtleber, Zhao, Raabe: Mater. Sc. Engin. A 336 (2002) 81

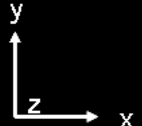
Crystal Mechanics FEM, grain scale mechanics (2D)



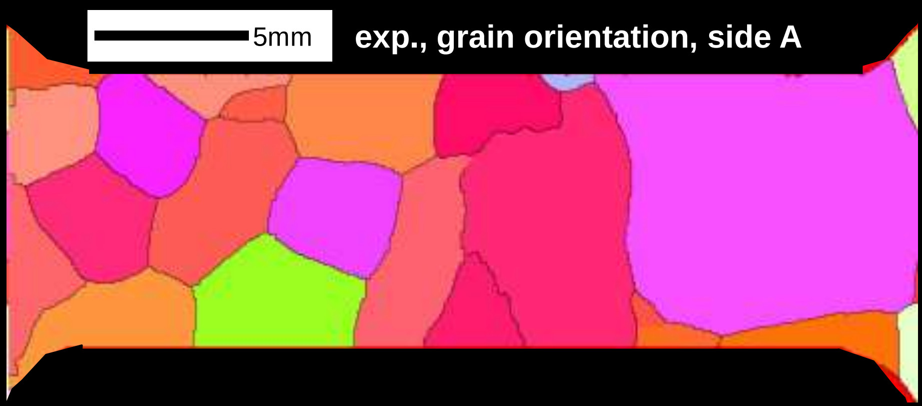


Experiment
(DIC, EBSD)
v Mises strain

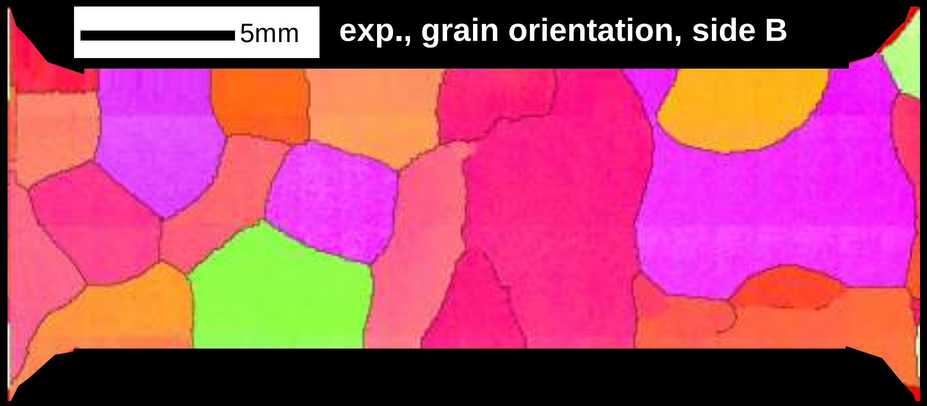
Simulation
(CP-FEM)
v Mises strain



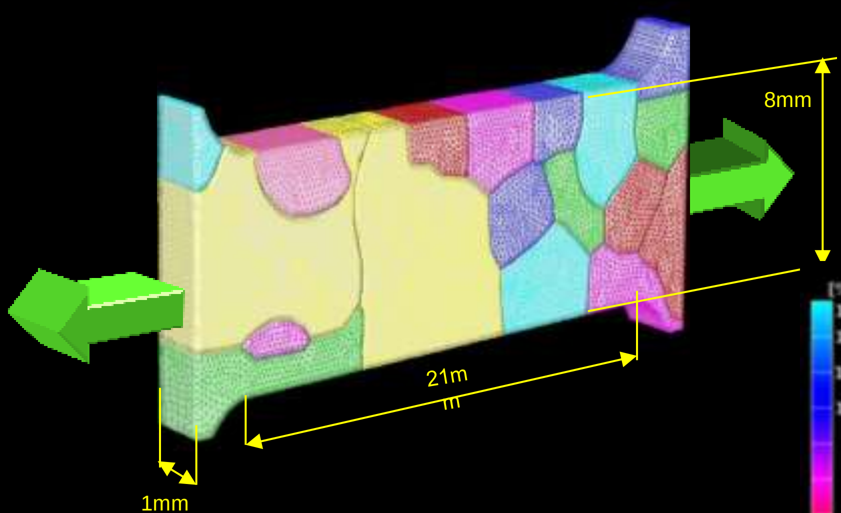
Crystal plasticity FEM, grain scale mechanics (3D Al)



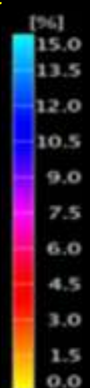
exp., grain orientation, side A

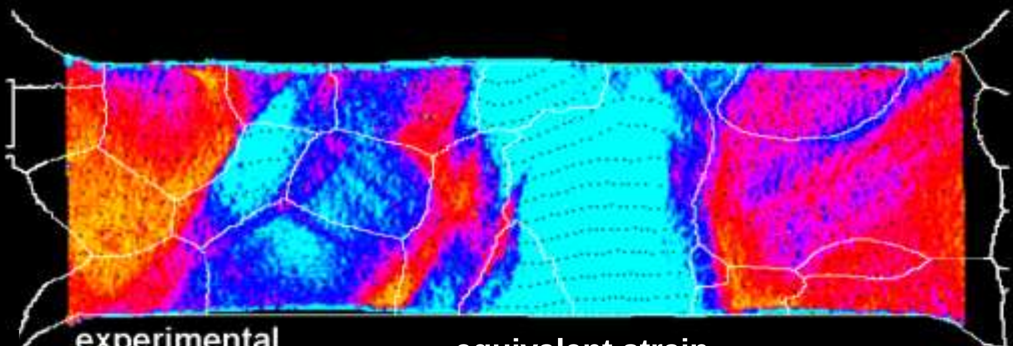


exp., grain orientation, side B

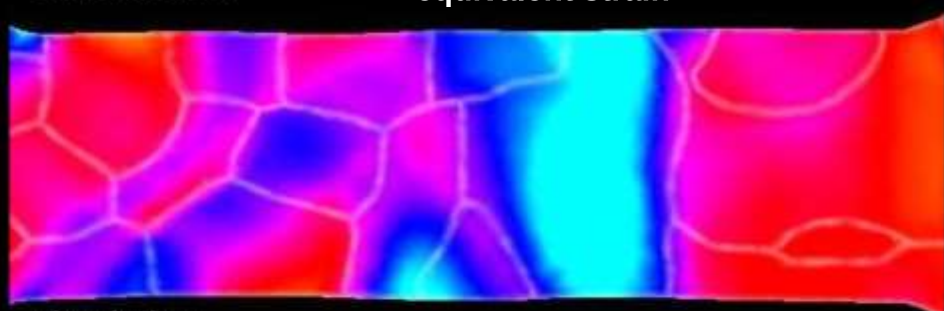


FE mesh



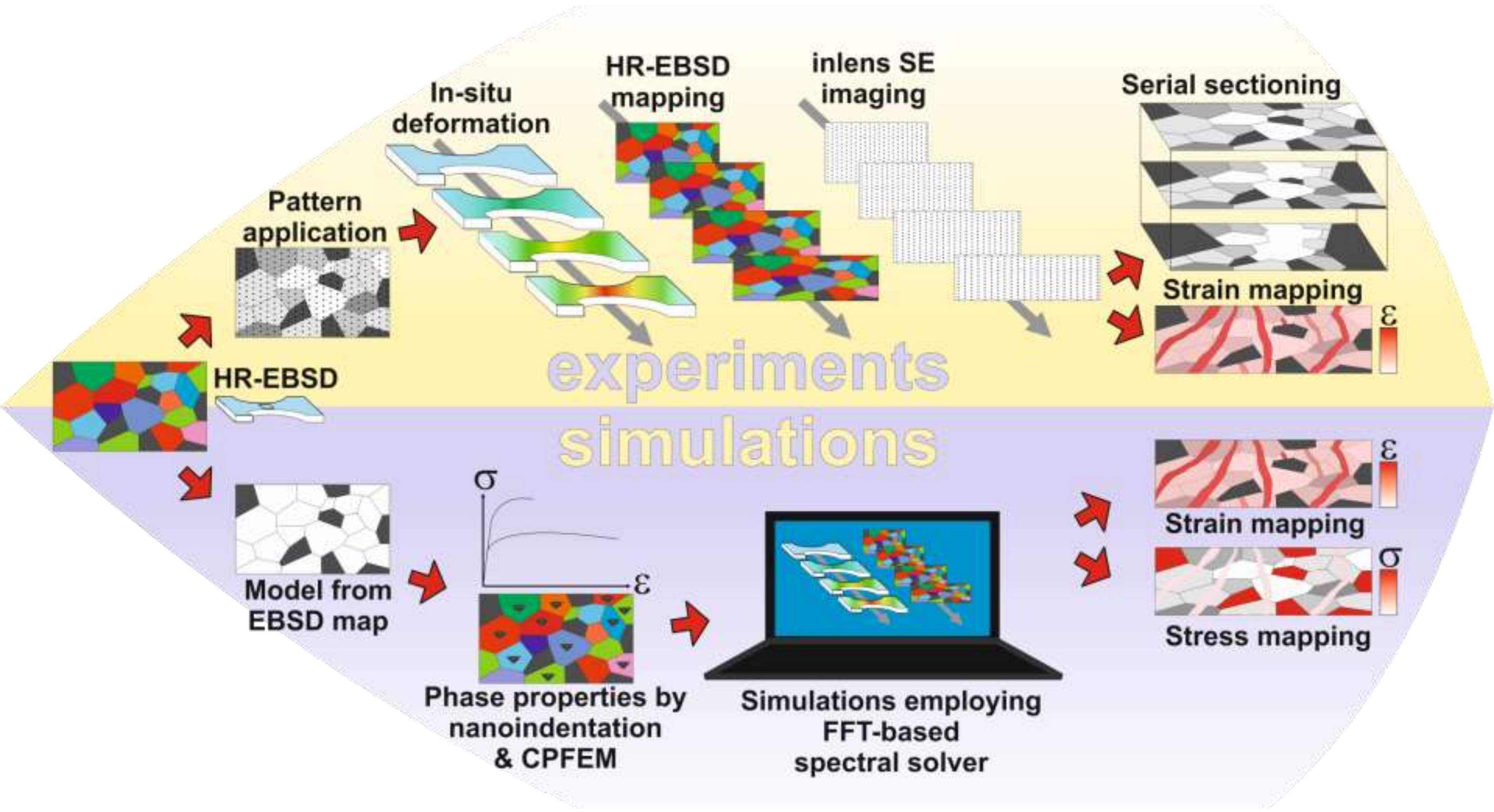


experimental equivalent strain

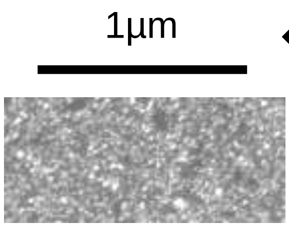


simulation equivalent strain

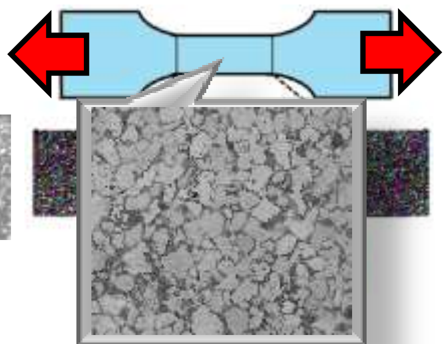
Zhao, Rameshwaran, Radovitzky, Cuitino, Roters, Raabe : Intern. J. Plast. 24 (2008)


In-situ deformation
HR-EBSD mapping
inlens SE imaging
Serial sectioning
Pattern application
Strain mapping
ε
HR-EBSD
experiments
simulations
σ
ε
Strain mapping
σ
Model from EBSD map
Phase properties by nanoindentation & CPFEM
Simulations employing FFT-based spectral solver
Stress mapping

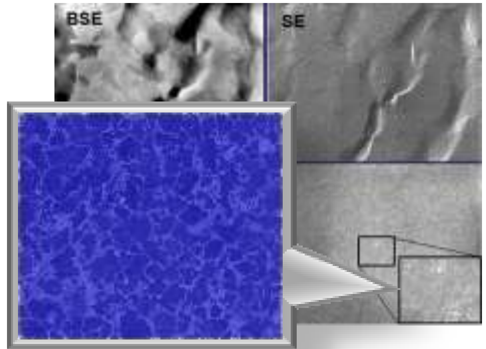
ICME applied to dual phase steel



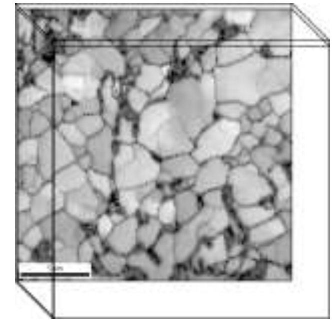
SiO_2 pattern



Deformation

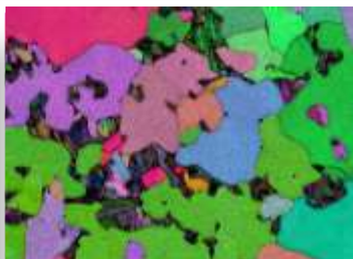


Imaging & DIC



Sectioning

Strain map

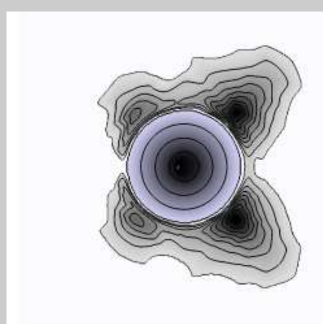


Experiments

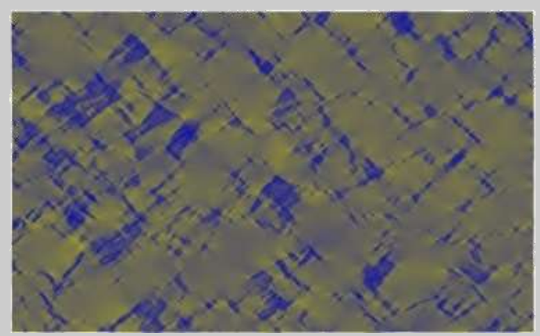
Simulations

Digital model

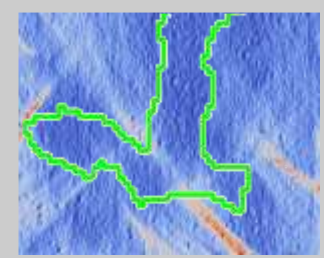
Indents



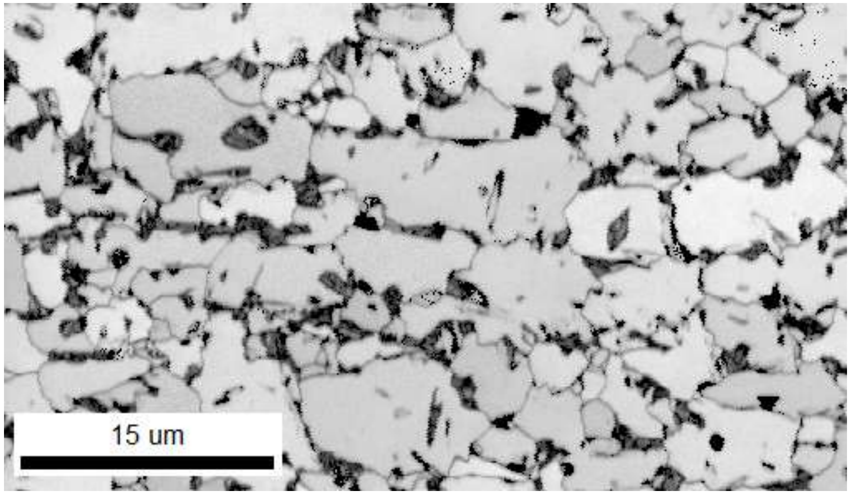
Spectral solver

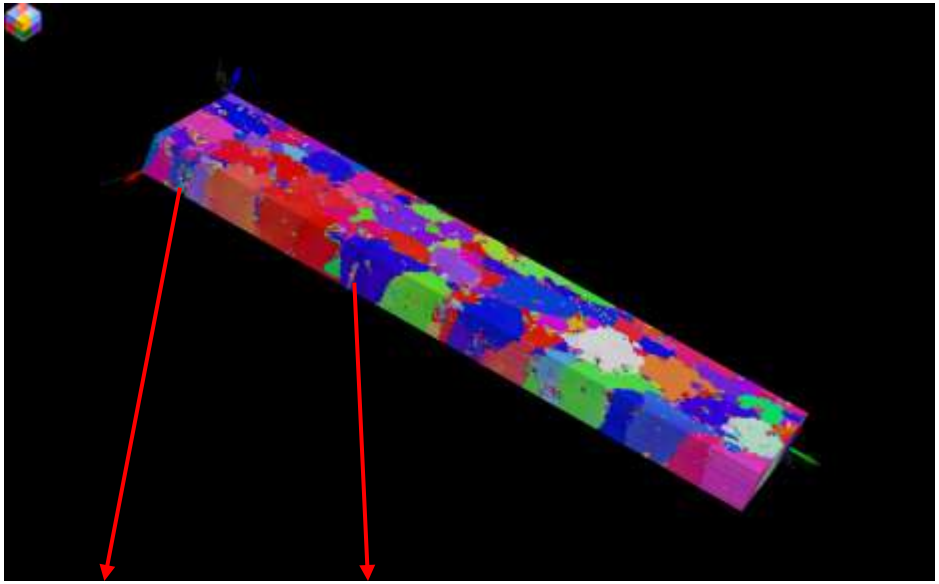


Strain map & stress map

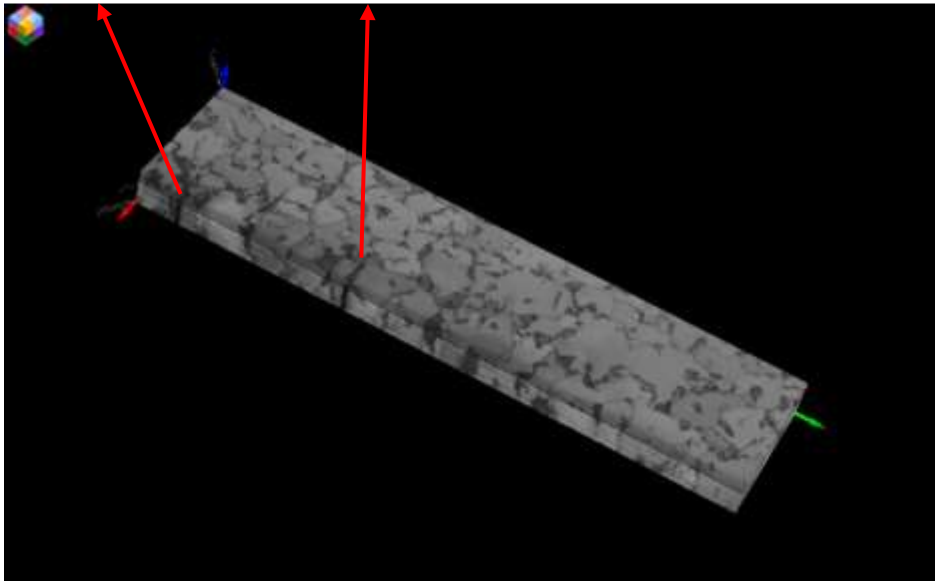


Real 3D Microstructure





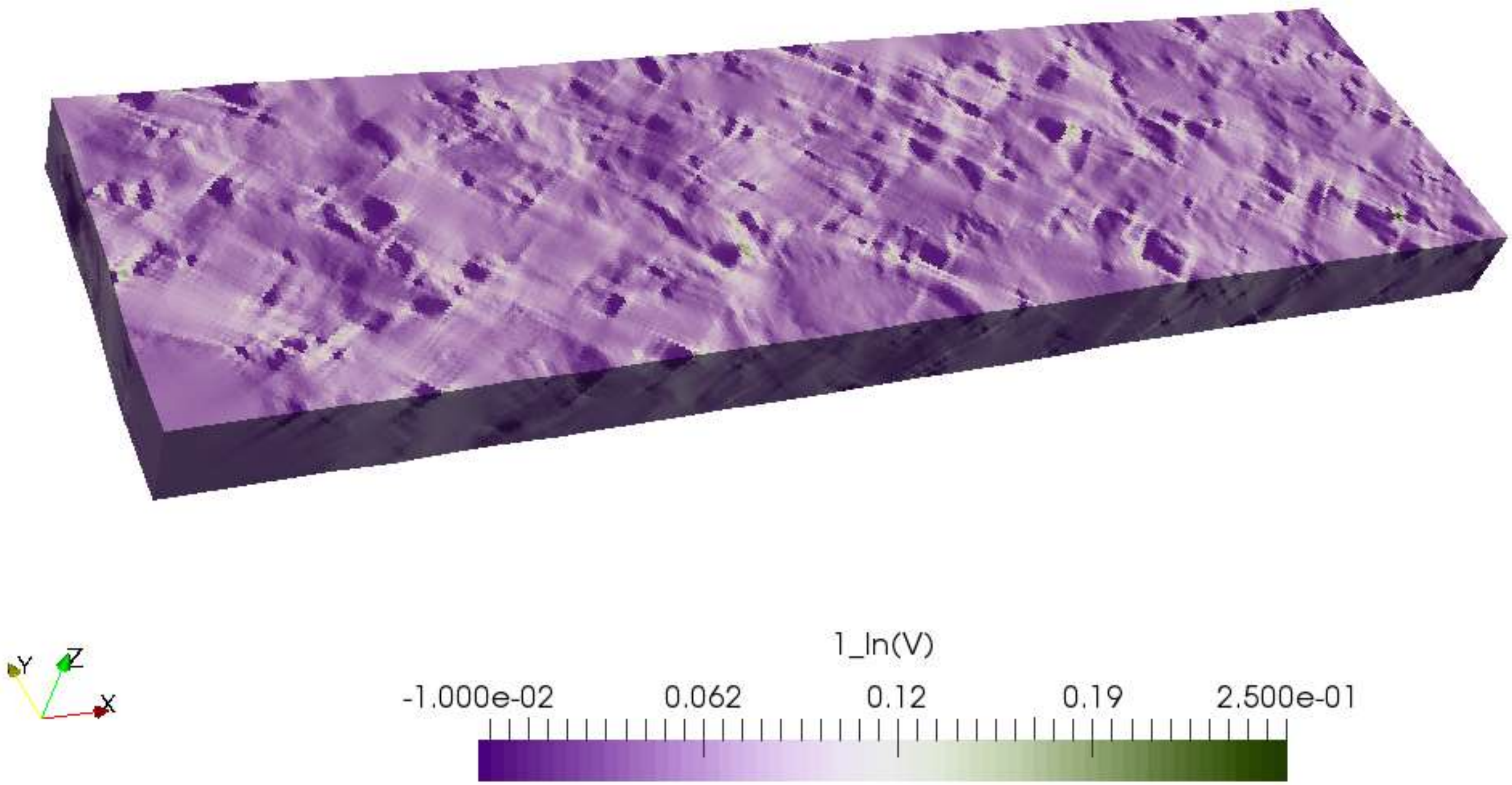
Marker lines act as a realignment reference



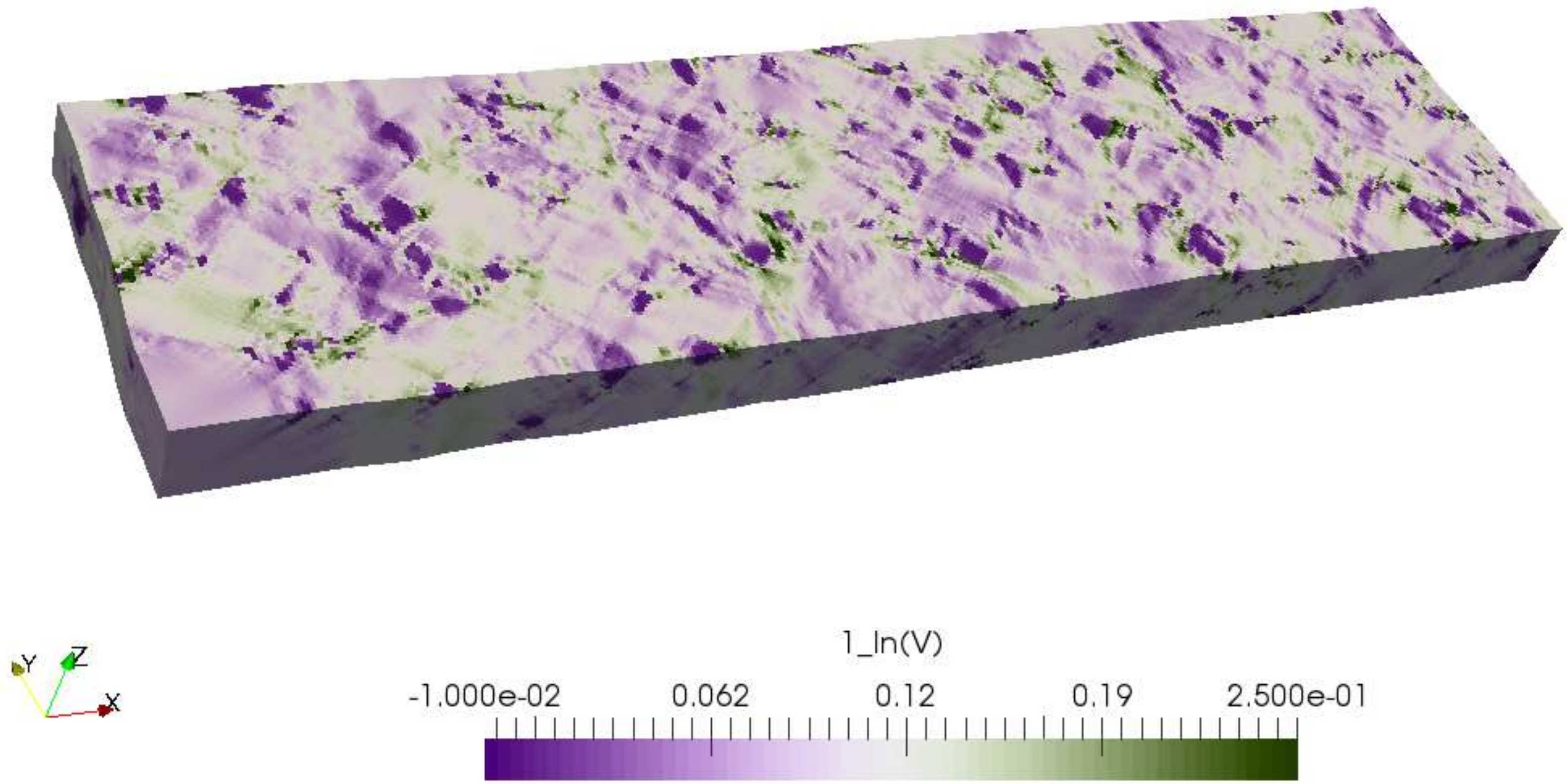
Average grain size: 5 µm
EBSD step size: 0,2 µm
EBSD scan size: 20 × 70 µm
Target polished thickness: 0,15 µm
Total slices number: 22

Experiment by Dayong An, MPIE

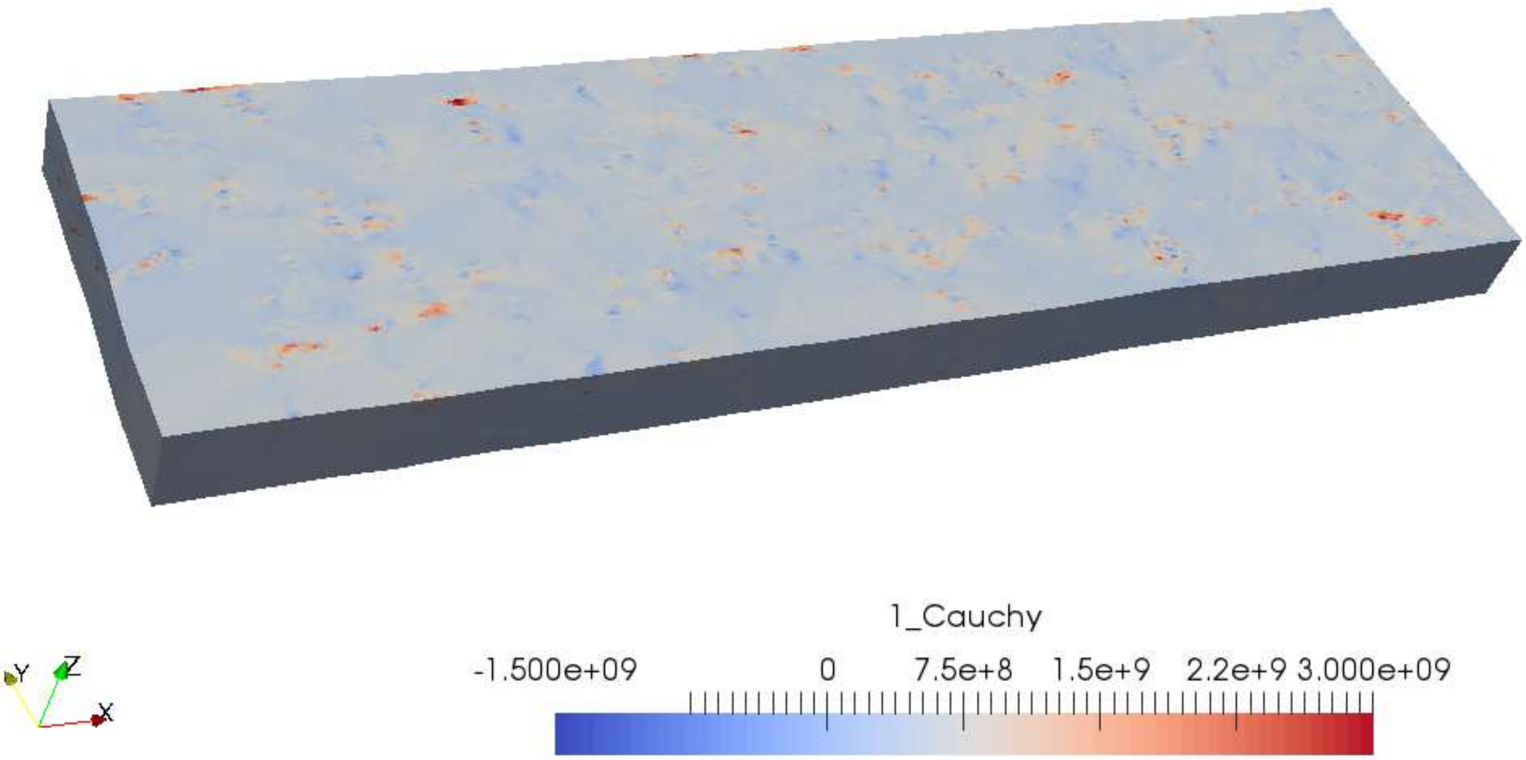
Real 3D Microstructure



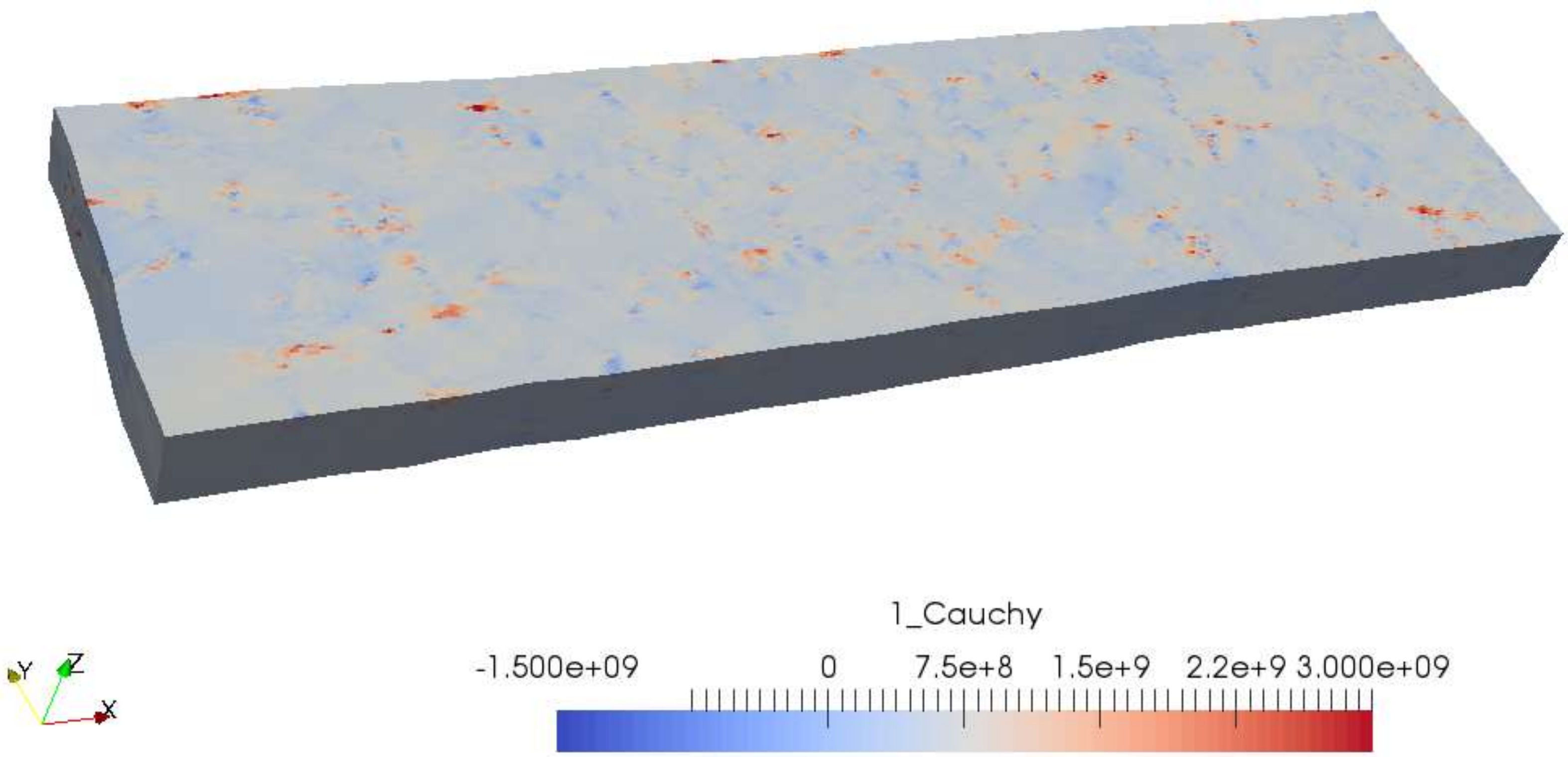
Real 3D Microstructure



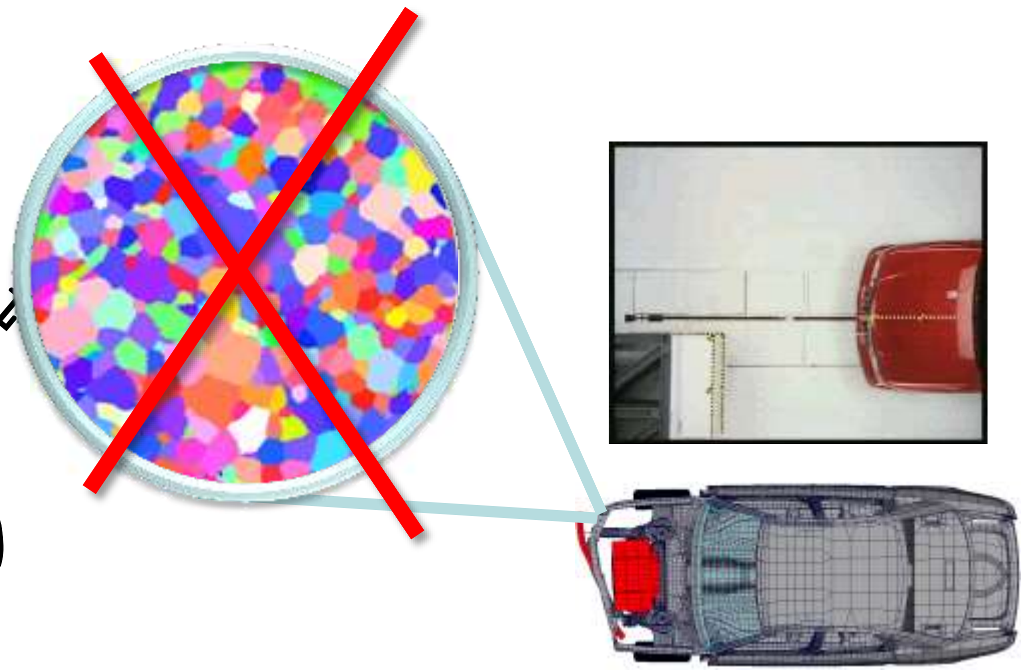
Real 3D Microstructure



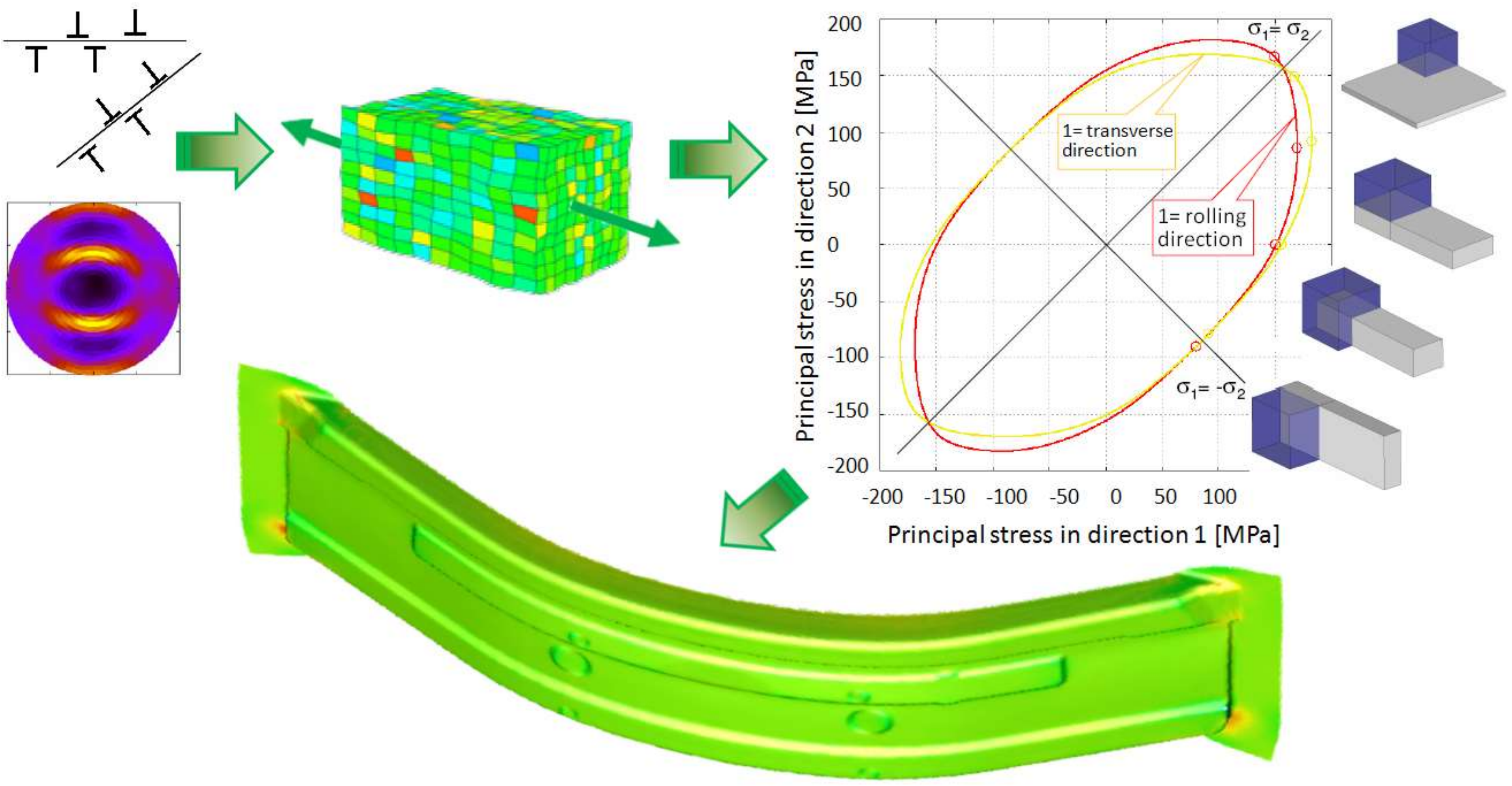
Real 3D Microstructure



too many grains

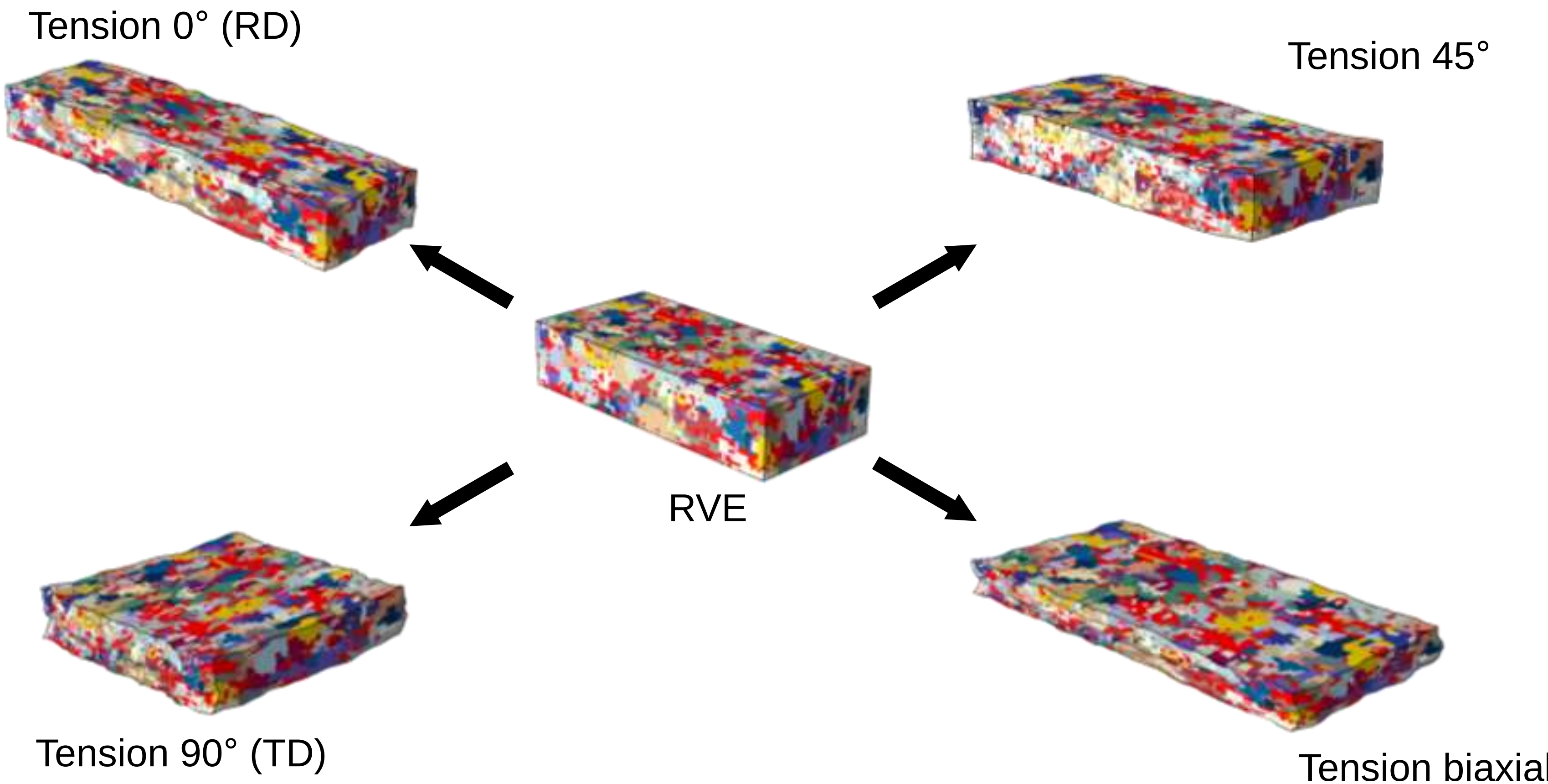


Numerical Laboratory: From CPFEM to yield surface (engineering)

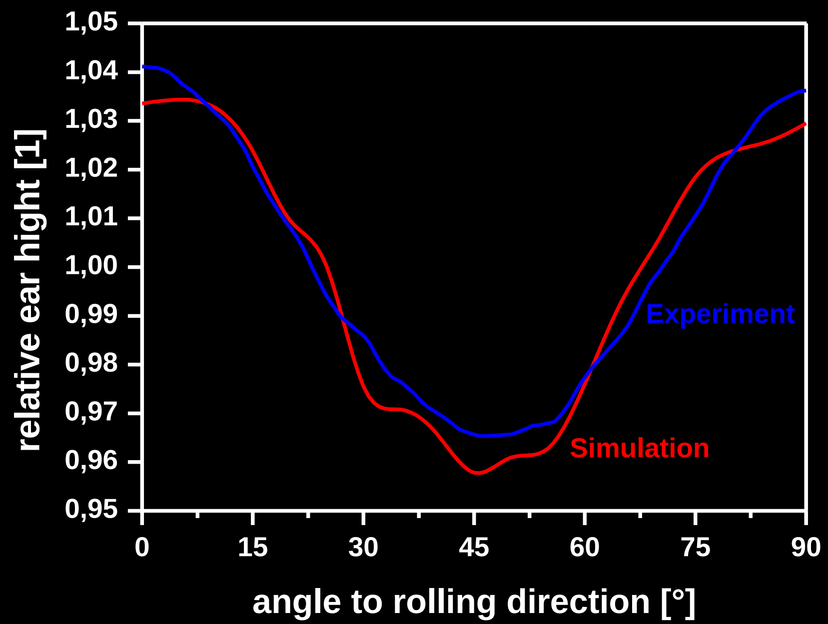


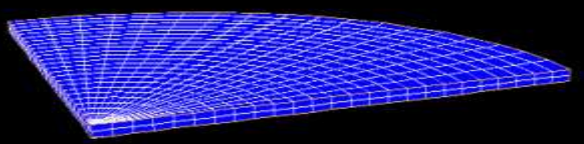
Kraska, Doig, Tikhomirov, Raabe, Roters, Comp. Mater. Sc. 46 (2009) 383

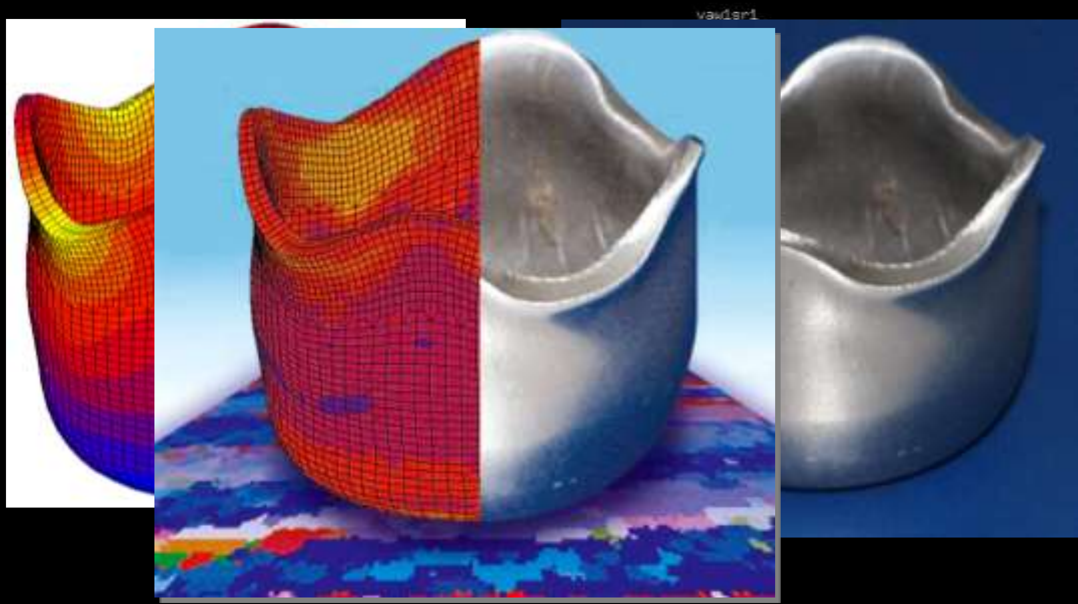
Representative Volume Element



Texture component crystal plasticity FEM for large scale forming

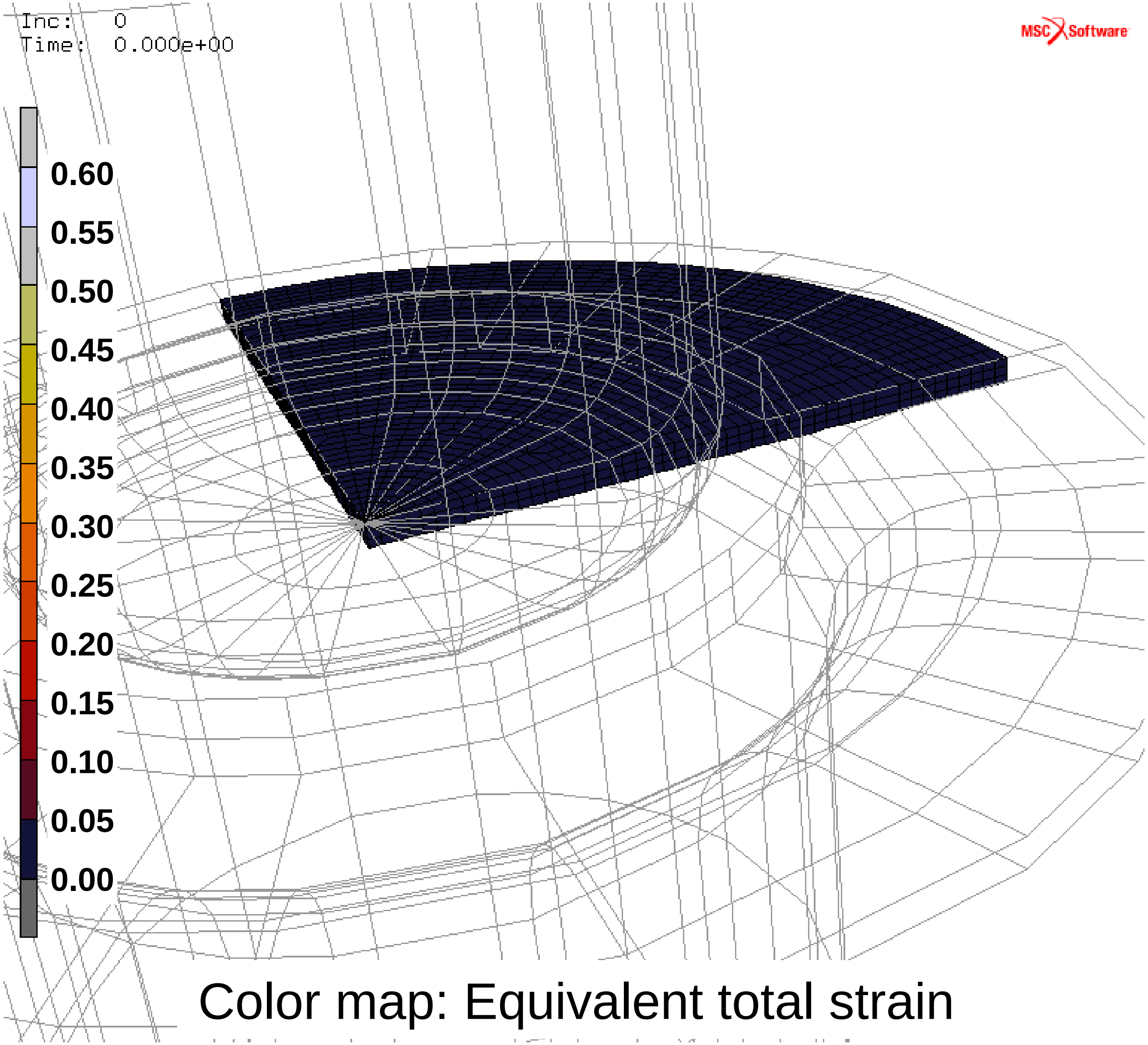






D. Raabe and F. Roters: Intern. J. Plast. 20 (2004) 339

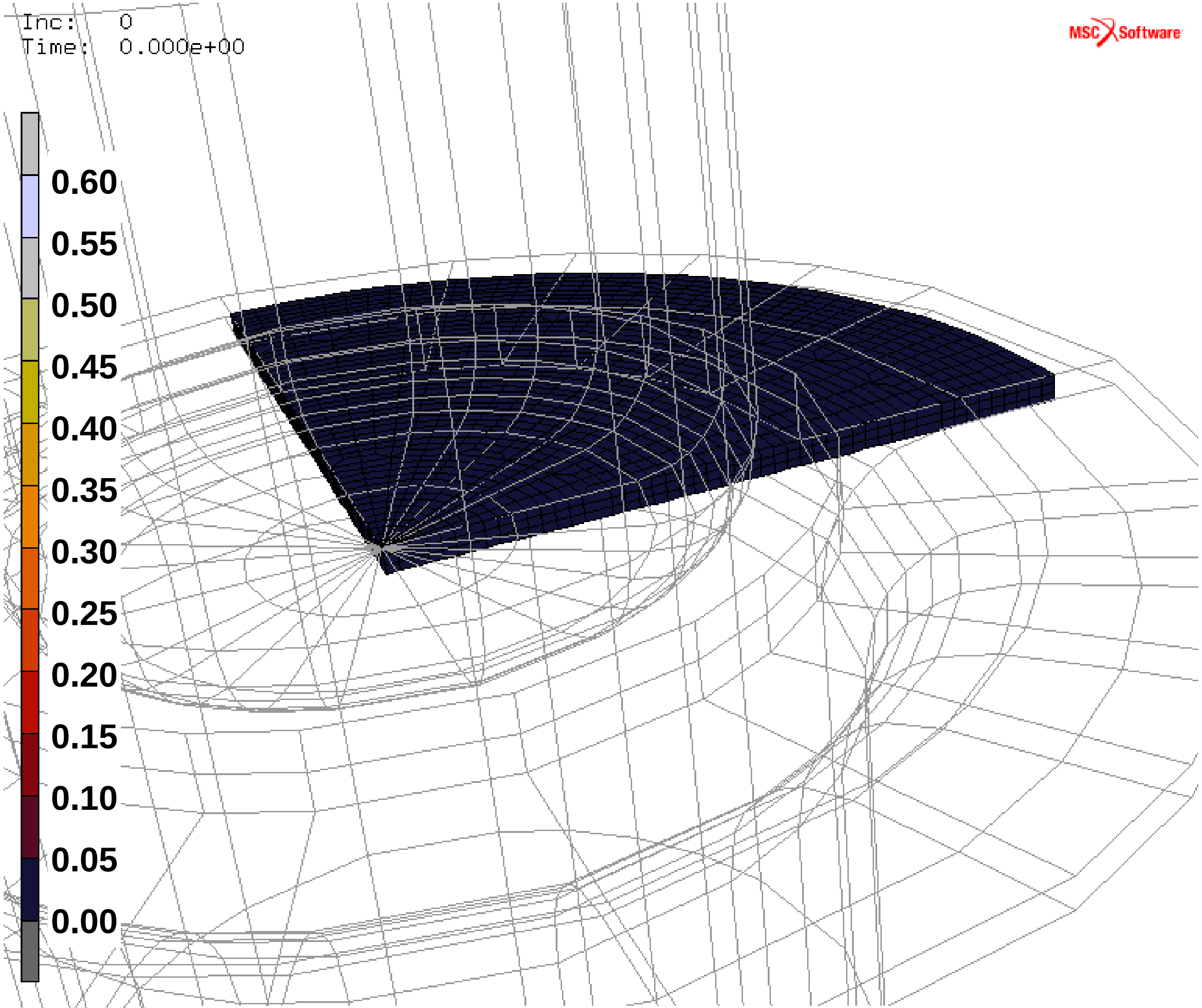
Simulation result: Taylor model



Color map: Equivalent total strain

Roters et al. Acta Mater.58 (2010)

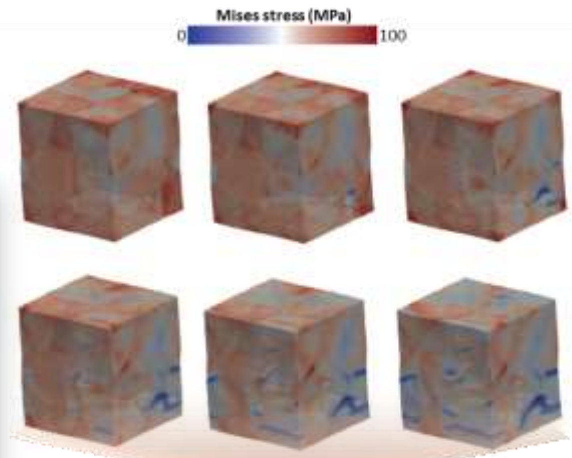
Simulation result: RGC scheme



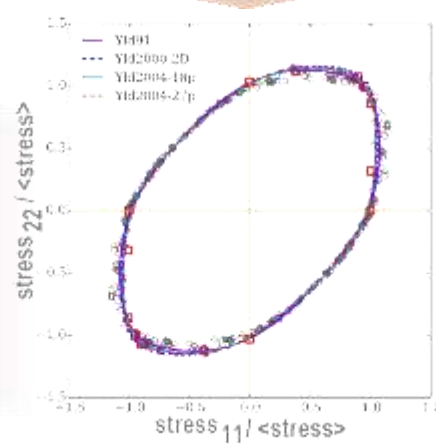
Color map: Equivalent total strain

Roters et al. Acta Mater.58 (2010)

Crystal plasticity & phase field:
Mechanics, damage, phase transformation, diffusion



- > 15 years of development
- > 50 man years of expertise
- > 50.000 lines of code
- Pre- and post-processing
- Blends with MSC.Marc and Abaqus
- Standalone (FFT) spectral solver
- Many user groups



http://DAMASK.mpie.de

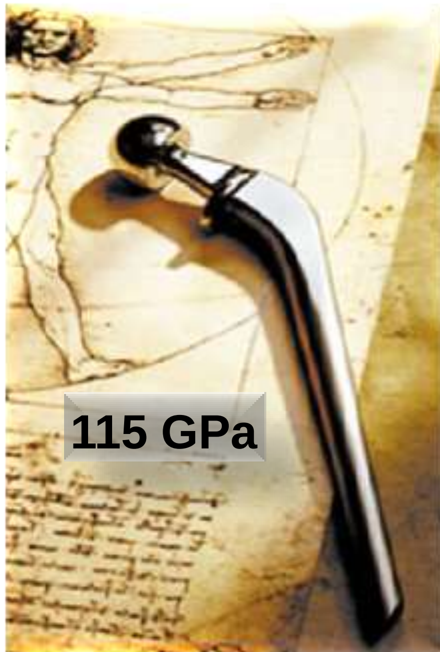
Overview

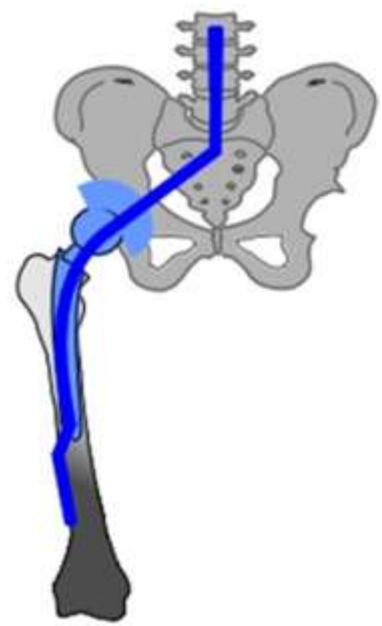
- **Some basic methods**
  - Atomistic
  - Monte Carlo
  - Dislocations
  - Polycrystal mechanics

- **Ab-initio informed constitutive models**
  - Elasticity: from DFT to Homogenization
  - Atomistically informed simulation: from APT to MD
  - From DFT to dislocation rate models and yield surfaces

DFT: Density Functional Theory; APT: Atom Probe Tomography; MD: Molecular Dynamics; RVE: Representative Volume Element; ICME: Integrated Computational Materials Engineering

Titanium implant materials with bcc structure





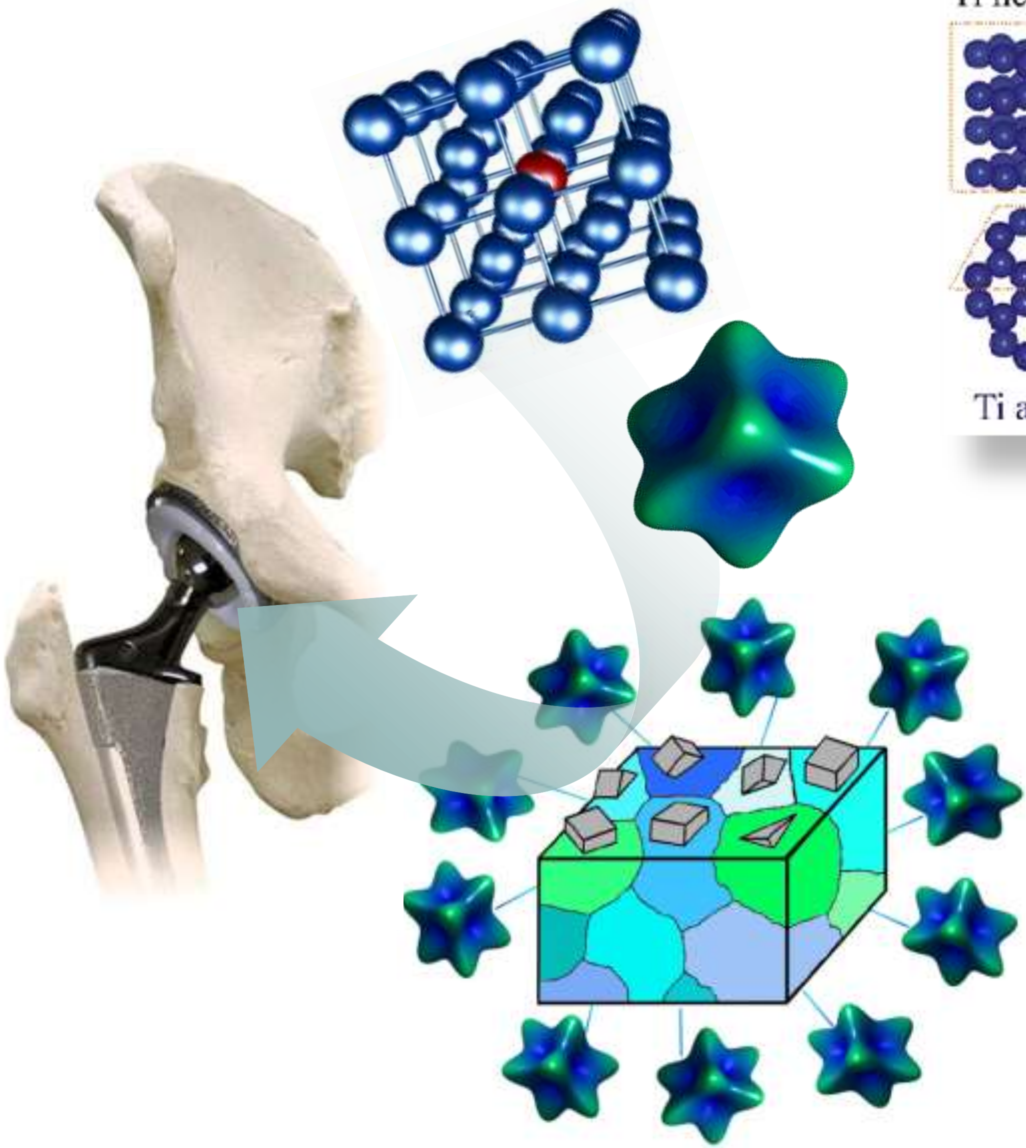
Stress shielding

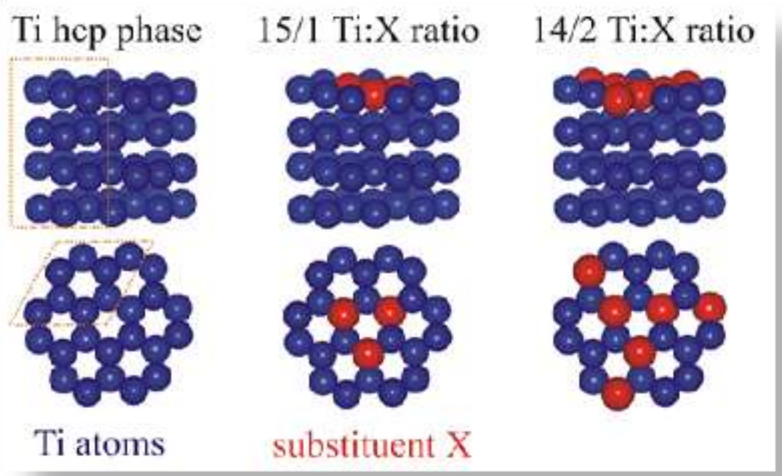
Elastic Misfit

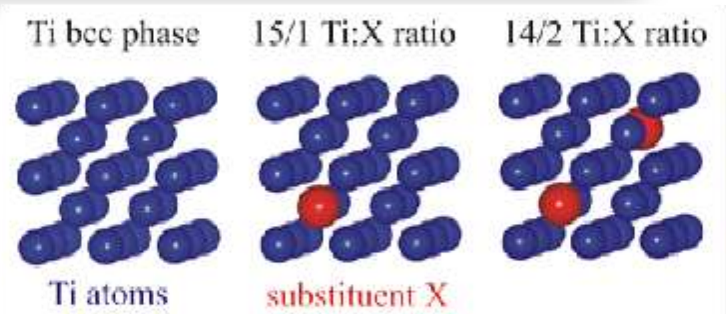
Bone mineral dissolution, abrasion

Raabe, Sander, Friák, Ma, Neugebauer: Acta Mater. 55 (2007) 4475

ab-initio Simulation of elastic stiffness



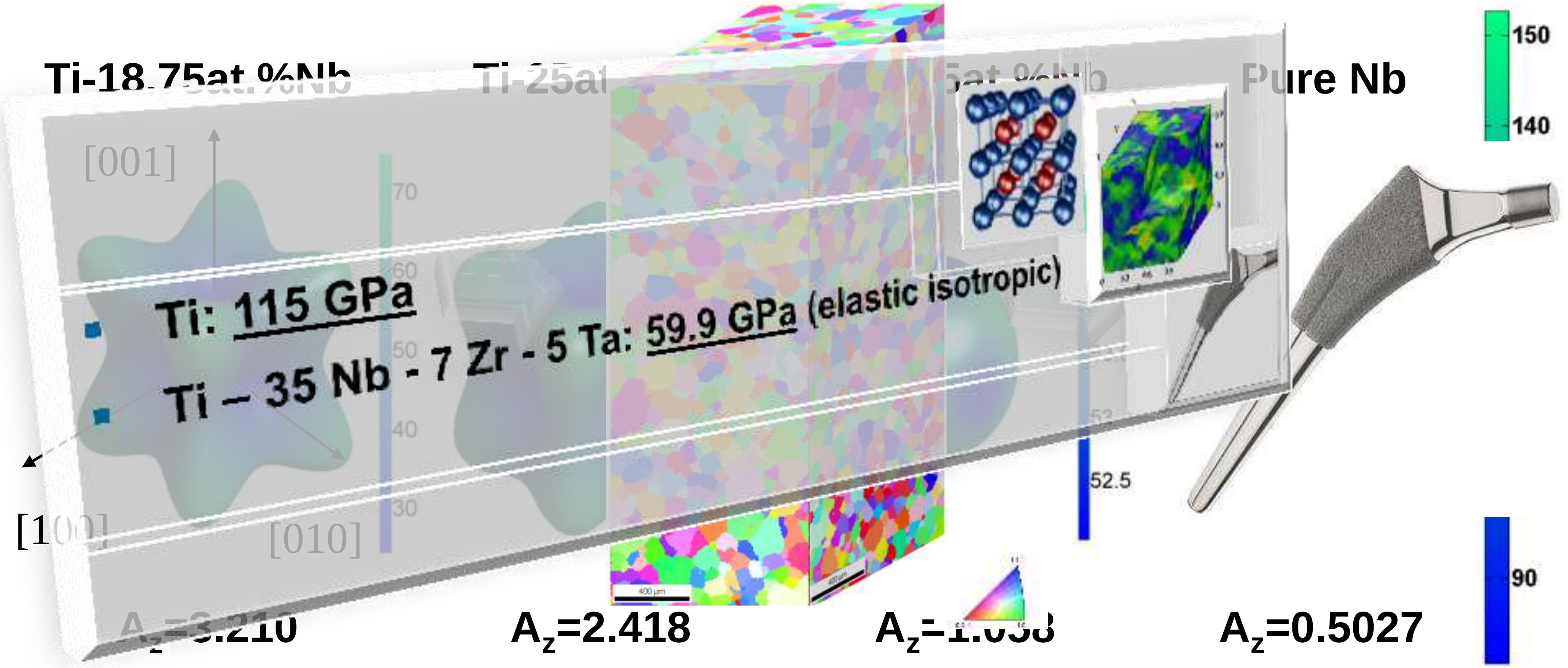




Raabe, Sander, Friák, Ma, Neugebauer: Acta Mater. 55 (2007) 4475

Ab initio alloy design: Elastic properties: Ti-Nb system

Young's modulus surface plots $A_z = 2\,C_{44}/(C_{11} - C_{12})$

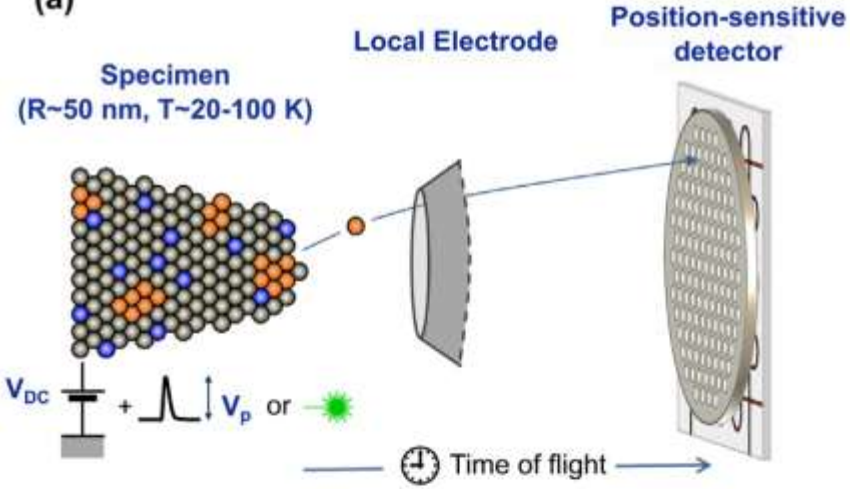


- Ti: 115 GPa
- Ti – 35 Nb - 7 Zr - 5 Ta: 59.9 GPa (elastic isotropic)

A_z=3.210 A_z=2.418 A_z=0.5027

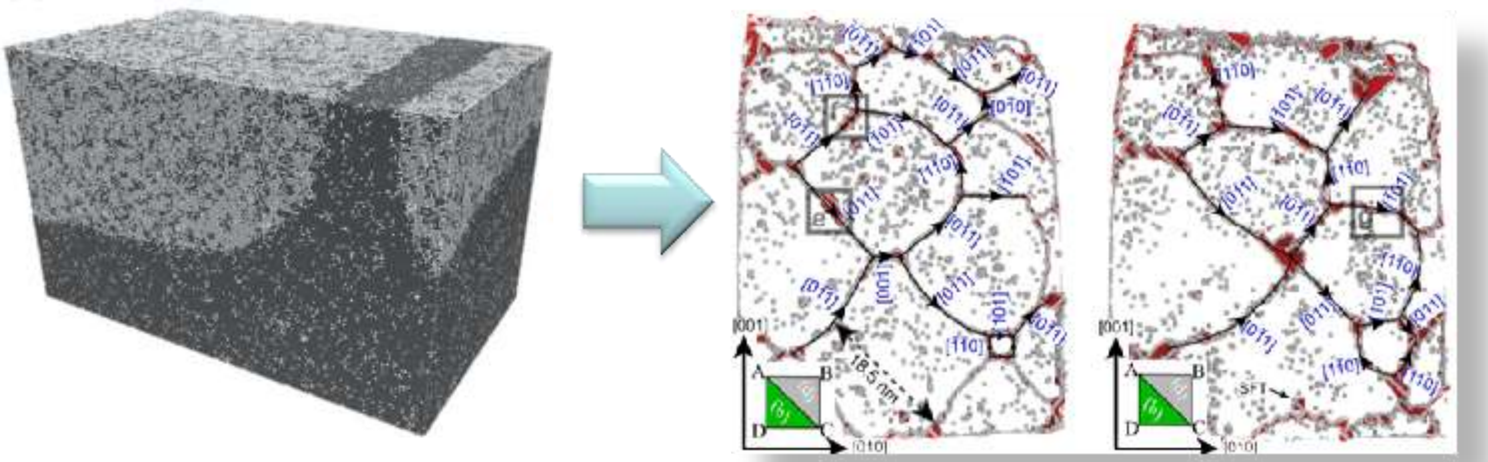
Ma, Friák, Neugebauer, Raabe, Roters: phys. stat. sol. B 245 (2008) 2642

(a)



(b)

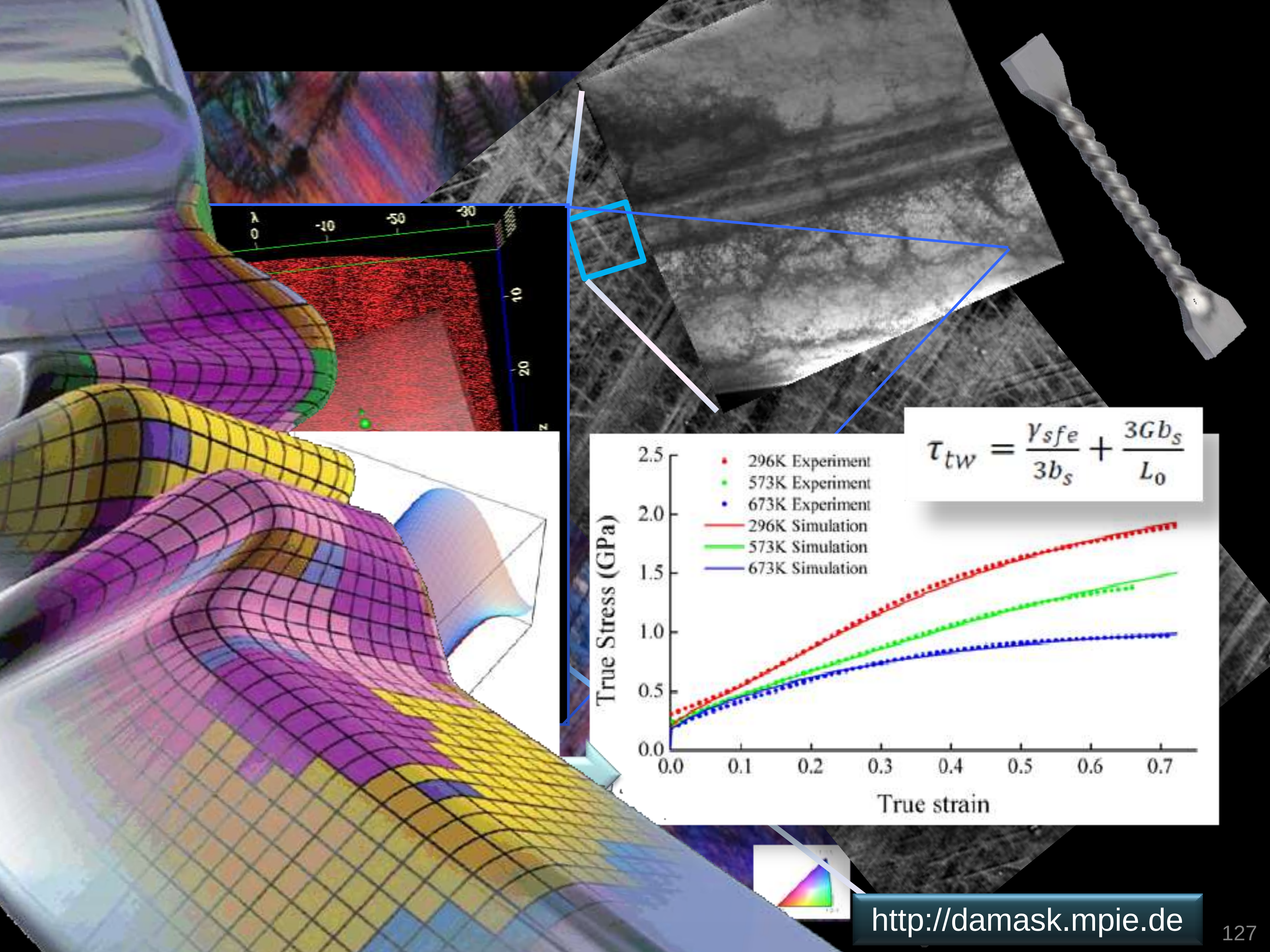
(e)



Prakash et al. (2015) Acta Materialia, 92

Example: 4th generation superalloys for turbine blades (SFB / TR 103)

Prakash, A. et al. Acta Materialia 92 (2015) 33



$\tau_{tw} = \frac{\gamma_{sfe}}{3b_s} + \frac{3Gb_s}{L_0}$
296K Experiment
573K Experiment
673K Experiment
296K Simulation
573K Simulation
673K Simulation
True Stress (GPa)
0.0
0.5
1.0
1.5
2.0
2.5
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
True strain
http://damask.mpie.de

The end ☺