Crystal Plasticity Modeling for FCC metals

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Cauchy Stress

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

Conservation of angular momentum leads to the symmetric property, i.e.,

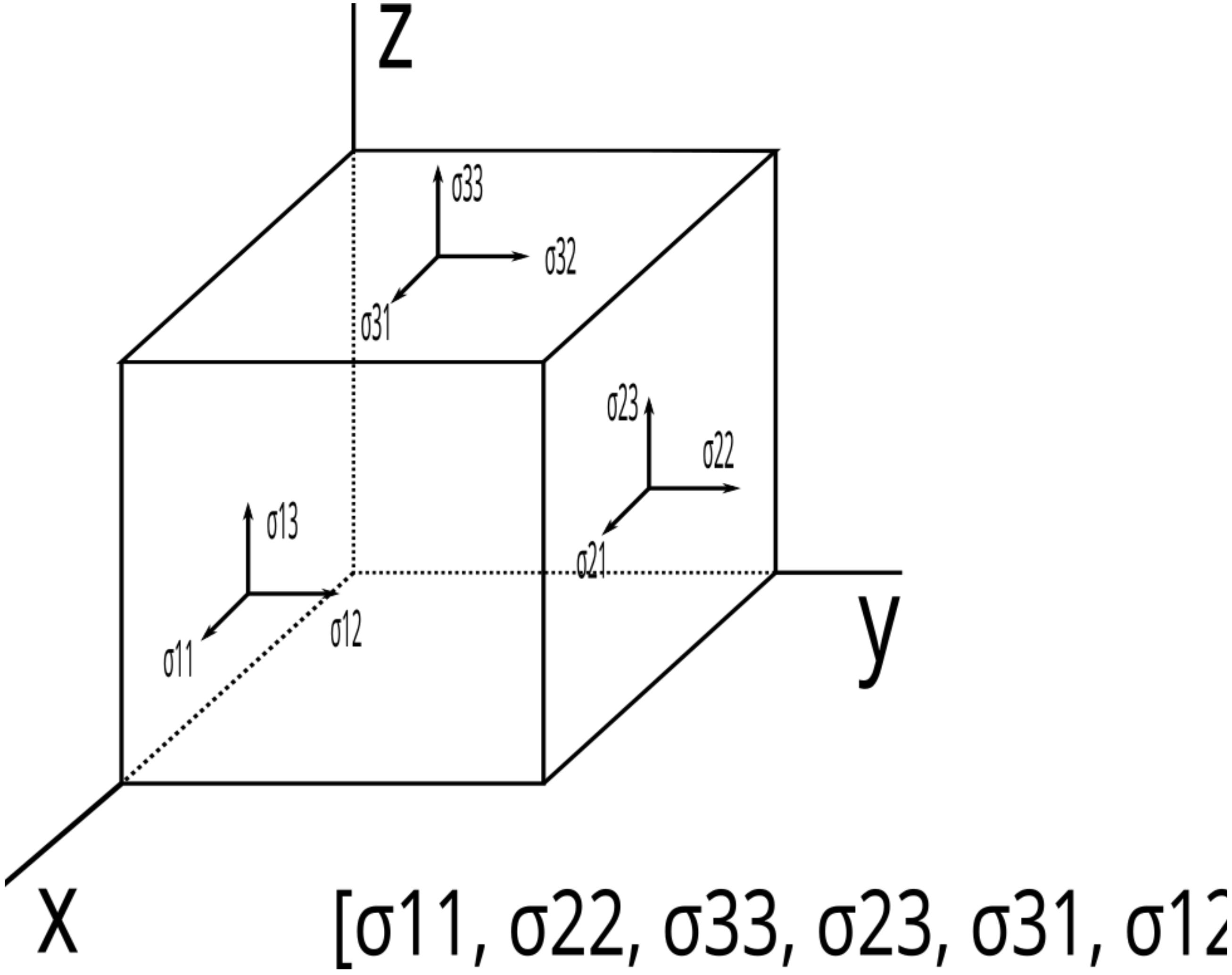
$$\sigma_{ij} = \sigma_{ji}$$

The surface traction t is related to the stress by the surface normal n,

$$\sigma_{ij} n_j = t_i$$

The surface traction can be decomposed to the components aligned with the normal and perpendicular to the normal. The traction projected to a direction m perpendicular to the normal is the shear stress component,

$$\tau = m_i t_i = m_i \sigma_{ij} n_j$$



Infinitesimal Strain

The infinitesimal strain is defined by the symmetric part of the displacement gradient, i.e.,

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

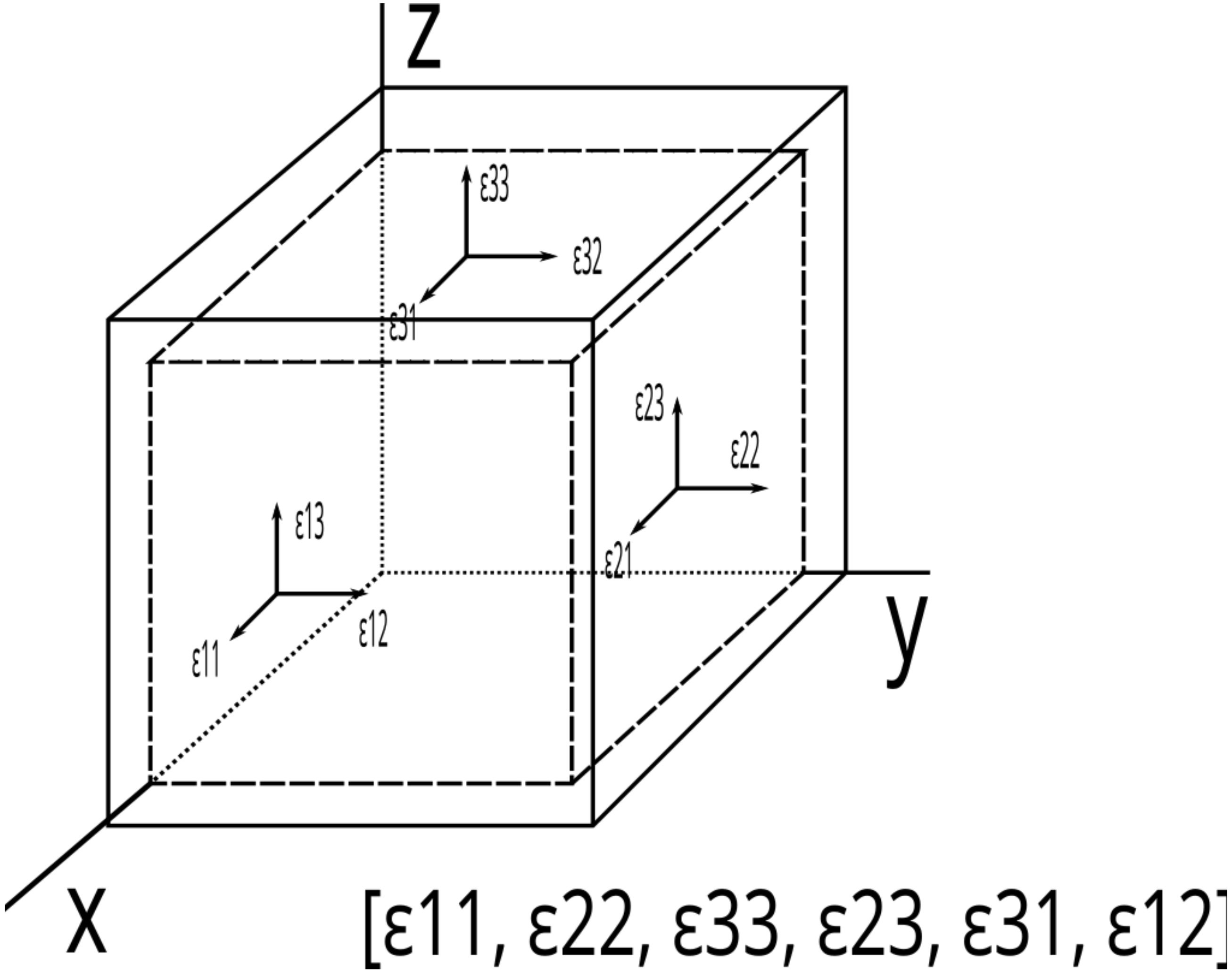
The strain can be decomposed to the dilatational part and the deviatoric part,

$$\varepsilon'_{ij} = \varepsilon_{ij} - \frac{1}{3}\varepsilon_{kk}\delta_{ij}$$

The deviatoric strain ε'_{ij} in these definition has the property,

$$\varepsilon'_{kk} = 0$$

For incompressible materials, the strain has five independent components.



Hooke's law

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$$

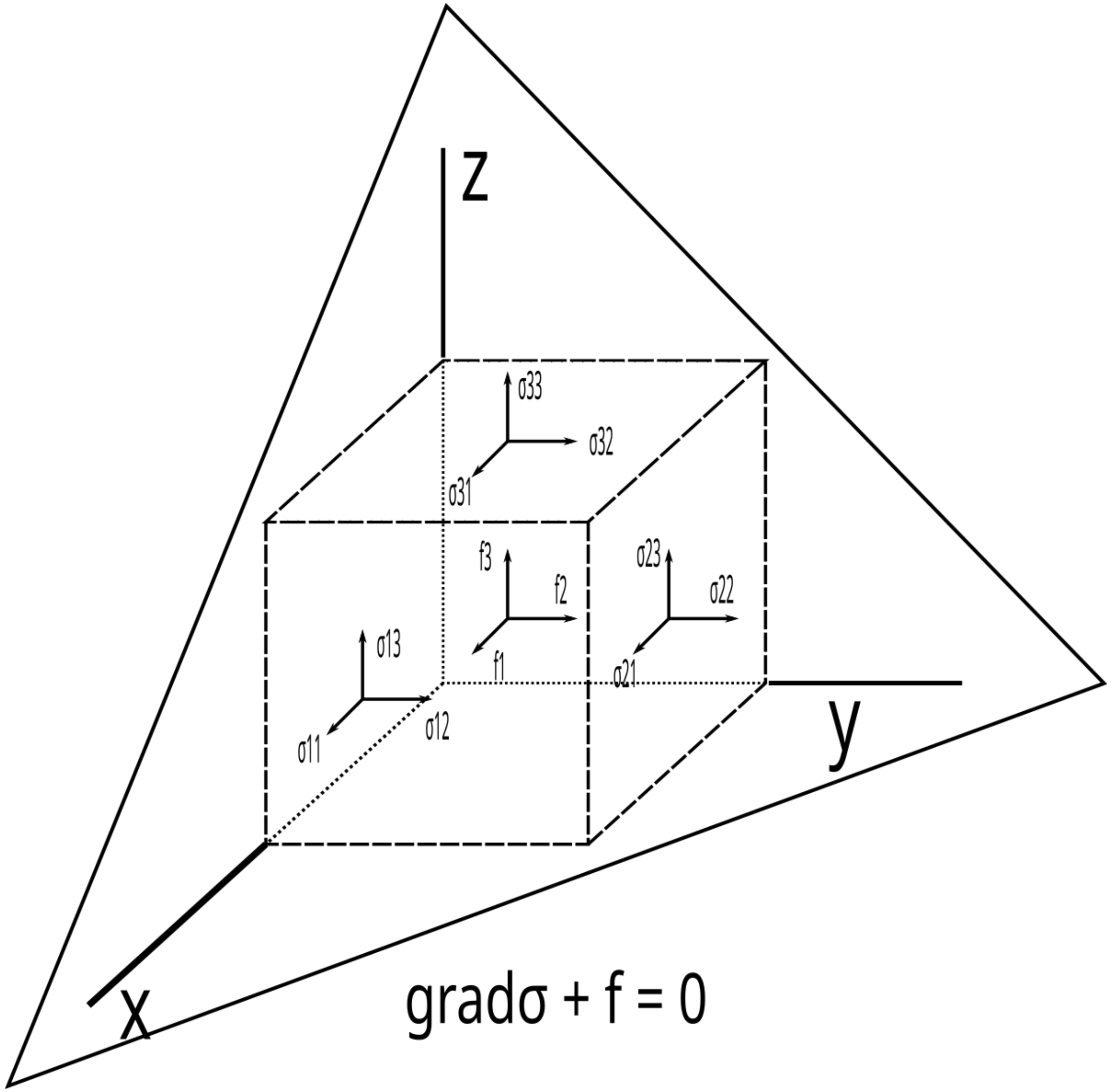
where c_{ijkl} are elastic constants. For cubic crystals,

$$\sigma_{11} = c_{11}\varepsilon_{11} + c_{12}\varepsilon_{22} + c_{12}\varepsilon_{33}$$
$$\sigma_{22} = c_{12}\varepsilon_{11} + c_{11}\varepsilon_{22} + c_{12}\varepsilon_{33}$$
$$\sigma_{33} = c_{12}\varepsilon_{11} + c_{12}\varepsilon_{22} + c_{11}\varepsilon_{33}$$
$$\sigma_{23} = 2c_{44}\varepsilon_{23}$$
$$\sigma_{31} = 2c_{44}\varepsilon_{31}$$
$$\sigma_{12} = 2c_{44}\varepsilon_{12}$$

In terms of the elastic constants for the isotropic materials,

$$\lambda + 2\mu = c_{11}$$
$$\lambda = c_{12}$$
$$\mu = c_{44} = \frac{1}{2}(c_{11} - c_{12})$$

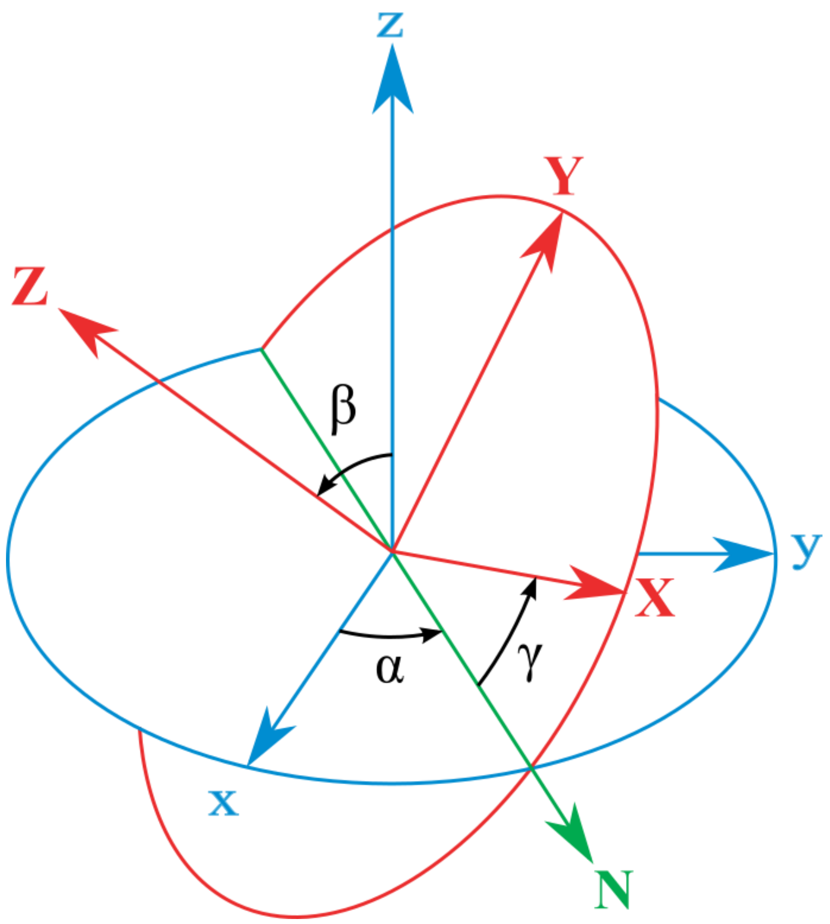
The shear modulus for a slip plane $\mu = \sqrt{c_{44}\frac{1}{2}(c_{11} - c_{12})}$



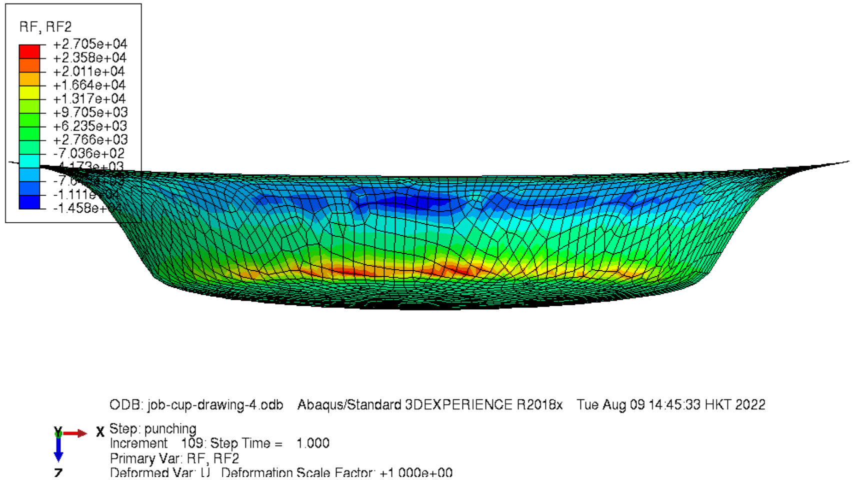
Isotropic Hooke's law

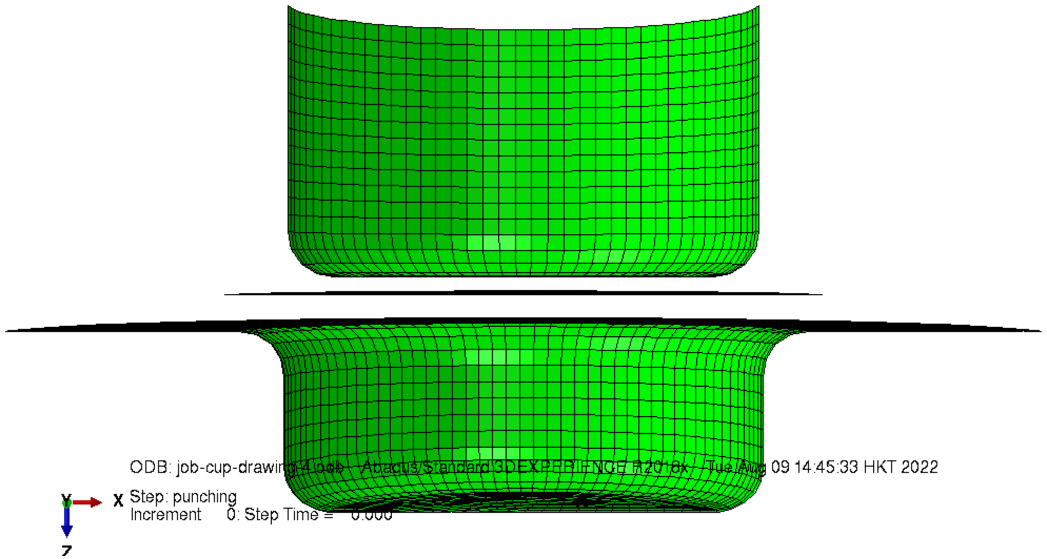
$$\varepsilon_{11} = \frac{1}{E}[\sigma_{11} - \nu(\sigma_{22} + \sigma_{33})]$$
$$\varepsilon_{22} = \frac{1}{E}[\sigma_{22} - \nu(\sigma_{11} + \sigma_{33})]$$
$$\varepsilon_{33} = \frac{1}{E}[\sigma_{33} - \nu(\sigma_{11} + \sigma_{22})]$$
$$\varepsilon_{23} = \frac{1}{2\mu}\sigma_{23}$$
$$\varepsilon_{31} = \frac{1}{2\mu}\sigma_{31}$$
$$\varepsilon_{12} = \frac{1}{2\mu}\sigma_{12}$$

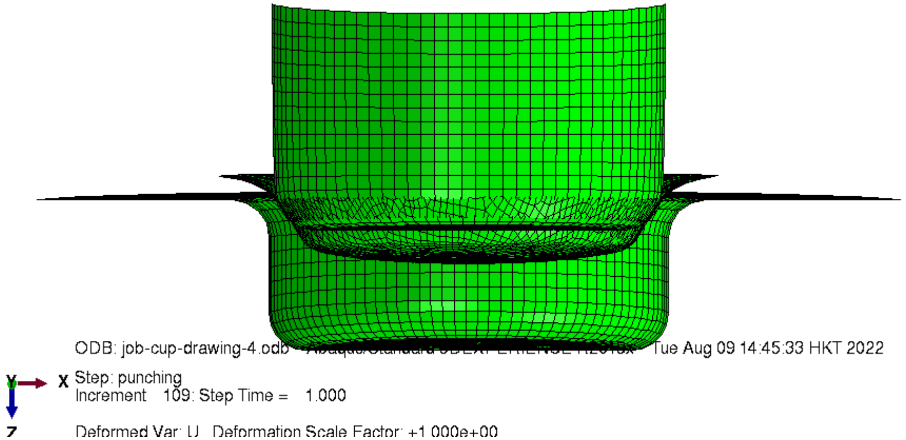
where the Young's modulus $E = 2\mu(1 + \nu)$. The Hooke's law is described on the ideal basis. If the orientation is considered, the transformation matrix (e.g. Euler angle) is required. In fact, the Young's modulus and the Lame's constant can be derived from the crystal symmetry.



A cup drawing example







Plastic strain

Consider the material deformation, the infinitesimal strain can be decomposed to the elastic and plastic parts,

$$\varepsilon_{ij} = \varepsilon_{ij}^{el} + \varepsilon_{ij}^{pl}$$

The plastic strain is of our interest and the elastic strain is usually neglected.

Here, the glide of slip plane is the mechanism of plastic deformation,

$$\varepsilon_{ij}^{pl} = \sum_{\beta=1}^{N} \gamma^{\beta} \mu_{ij}^{\beta}$$

where μ_{ij}^{β} characterized the slip plane and γ^{β} is the simple shear strain. In detail,

$$\mu_{ij}^{\beta} = \frac{1}{2}(m_i n_j + m_j n_i)$$

where m represents the slip direction and n represents the plane normal.

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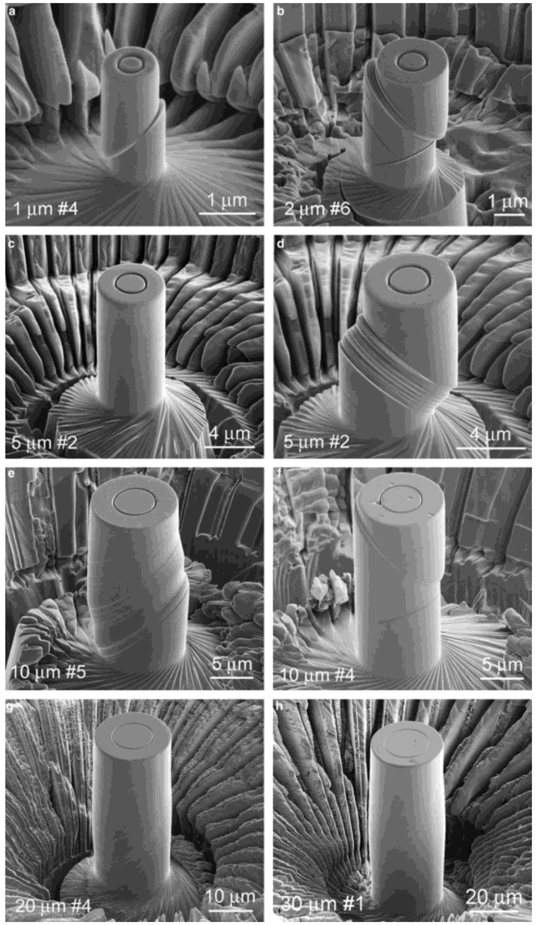

Fig. 4. SEM images of microcrystals: (a) 1 l m diameter sample after test showing intense localized shear; (b) 2 l m diameter sample after 56% shear showing activation of second slip plane; (c) 5 l m diameter sample before deformation; (d) sample shown in (c) after 90% compressive shear deformation; (e) and (f) 10 l m diameter samples after 9.6% and 12% shear strain, respectively; (g) and (h) 20 and 30 l m diameter samples after 20.5% and 17.% shear strain, respectively.

FCC Metals

The face-centered-cubic (FCC) metals (e.g. Aluminum) has 12 glide systems represented by a tetrahedron ABCD.

For a single crystal, 1~3 slip systems are active to perform simple shear test,

$$\varepsilon_{ij}^{pl} = \sum_{\alpha=1}^{3} \gamma^{\alpha} \mu_{ij}^{\alpha}$$

The applied shear stress is

$$\tau^{\alpha} = \sigma_{ij} \mu_{ij}^{\alpha}$$

and the total plastic strain is the summation of all the active slip systems,

$$\gamma = \sum_{\alpha=1}^{3} |\gamma^{\alpha}|$$

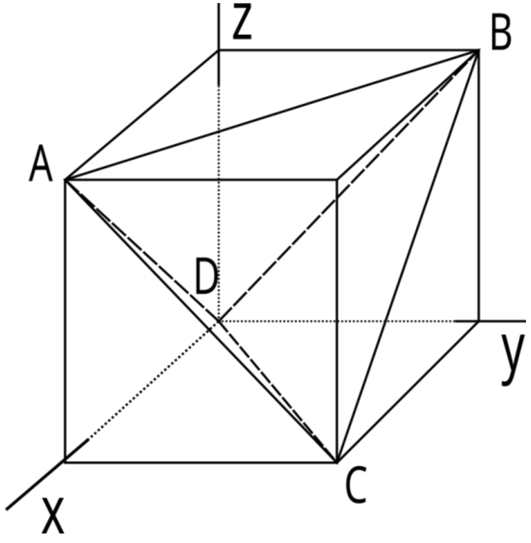

Figure 1

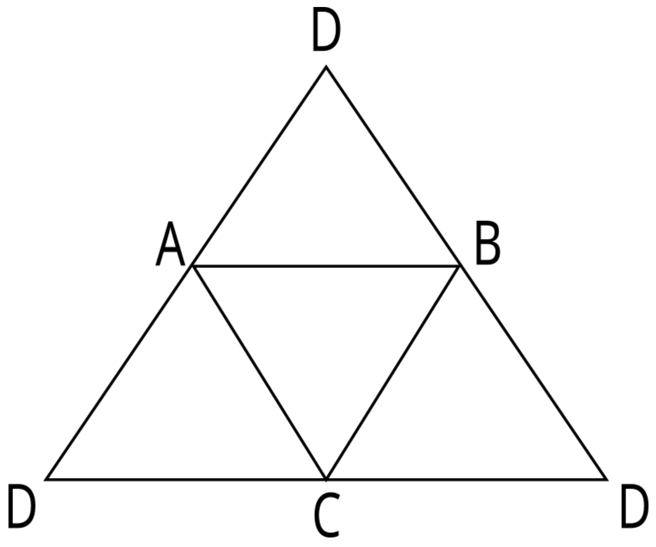

Figure 2

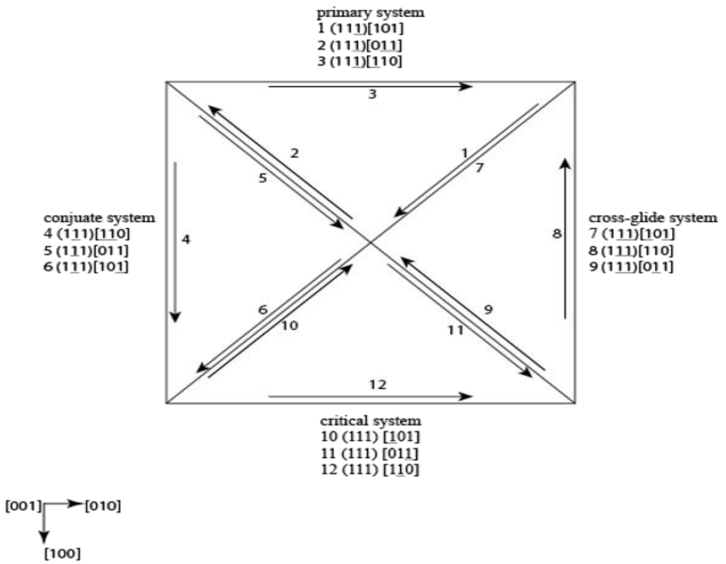

Figure 3

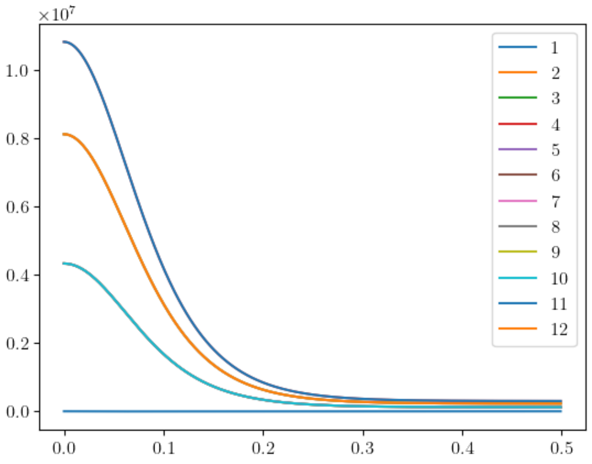

Figure 4

Simple shear test

The stress and strain of a simple shear test can be written as

$$\sigma_{ij} = \begin{bmatrix} 0 & \tau & 0 \\ \tau & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

and

$$\varepsilon_{ij} = \frac{1}{2}\begin{bmatrix} 0 & \gamma & 0 \\ \gamma & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

The constitutive relation $\tau = \tau(\gamma)$ is written implicitly in the slip rate form

$$\dot{\gamma}^{\alpha} = H_{\alpha\beta}^{-1}(\gamma)\dot{\tau}^{\beta}$$

where $H_{\alpha\beta}(\gamma)$ are the hardening coefficients.

The flow curves on the right hand side are the size effect of nanopillars, we will model its bulk behavior.

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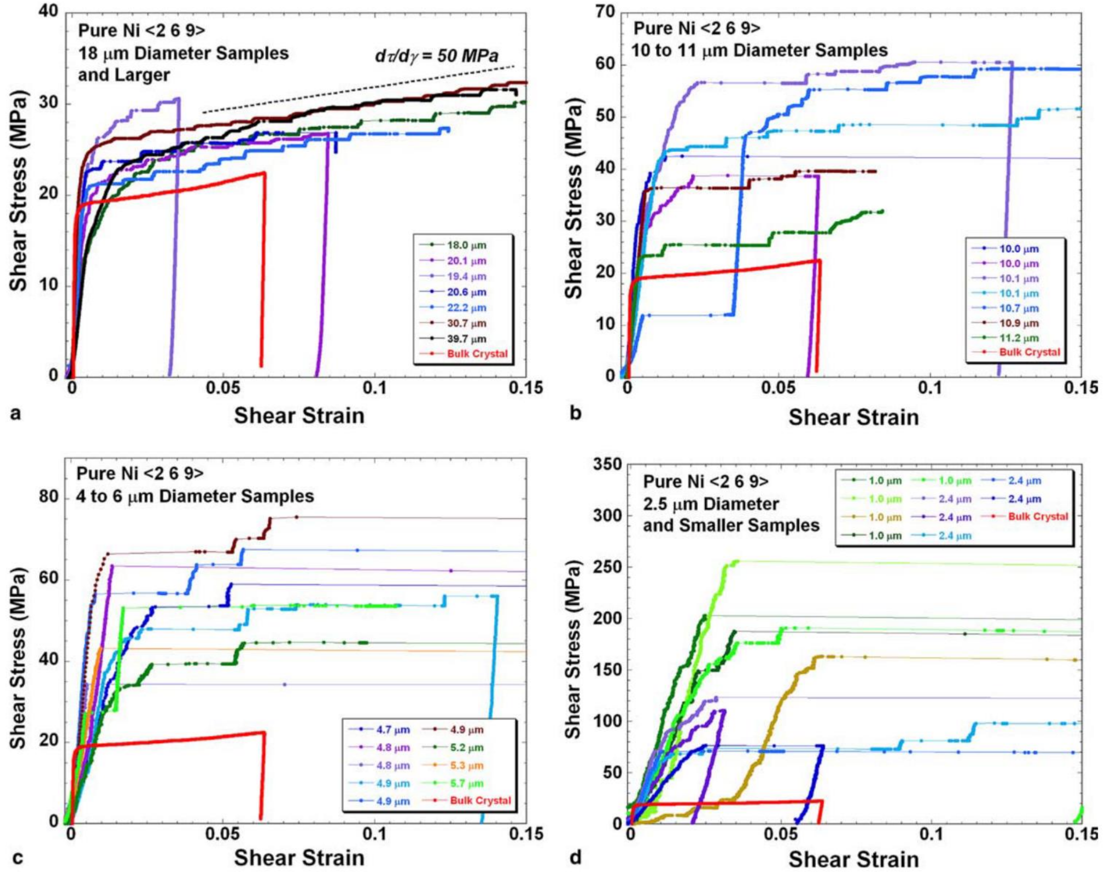
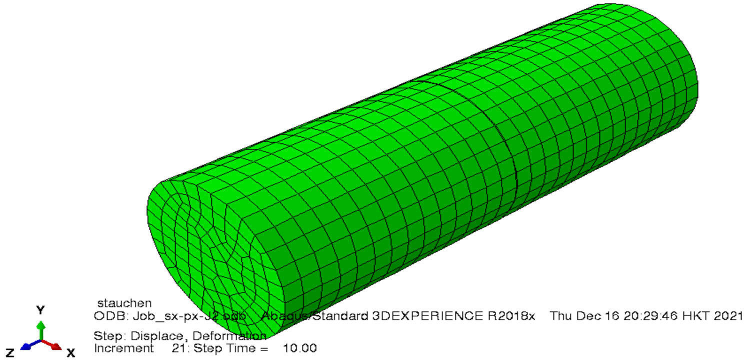
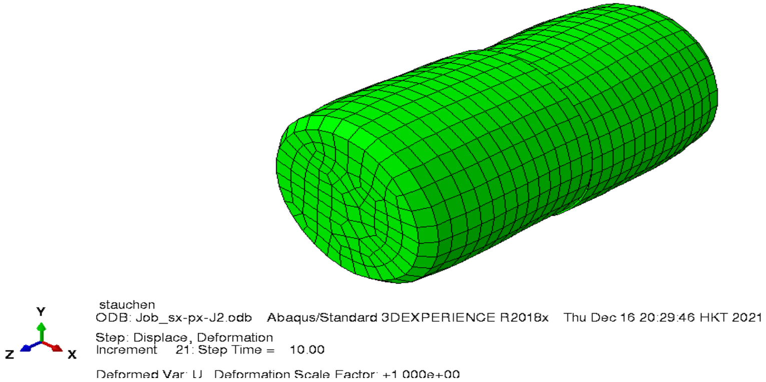


Fig. 3. Shear stress versus shear strain plots grouped by sample diameter: (a) 18 μm and greater; (b) 10–11 μm; (c) 4–6 μm; and (d) 2.5 μm and smaller. Note comparisons to the stress–strain curve from macroscopic crystal. Also, curves are truncated at 15% strain for clarity.

A micropillar compression example ($20\mu m$)



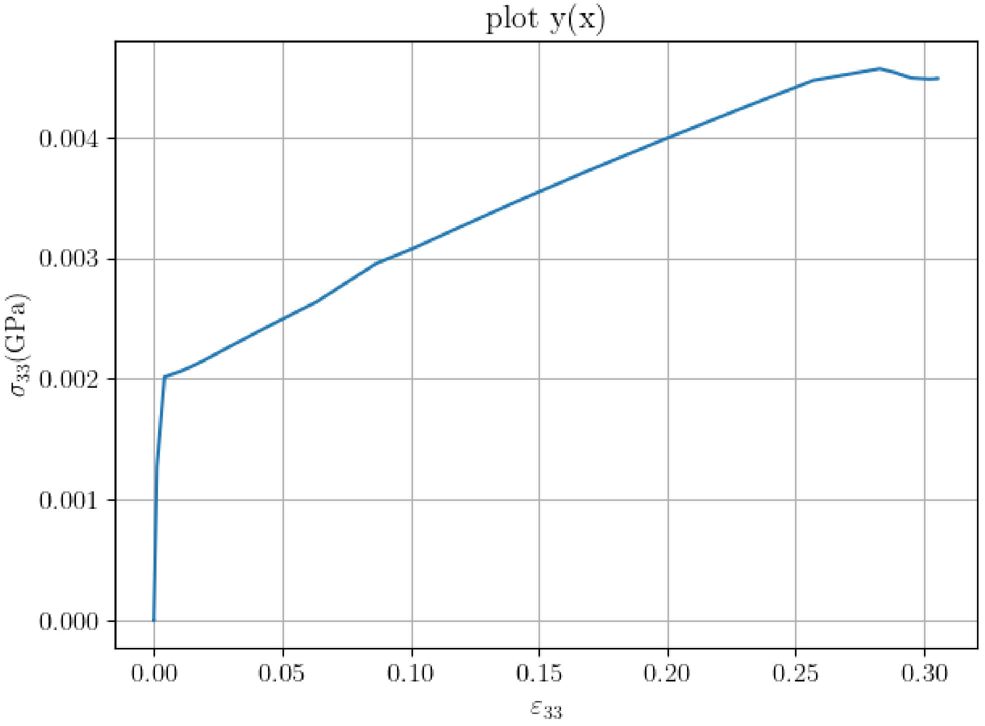


Young's modulus E = 2.0 Gpa	Poisson's ratio nu=0.3
Yield stress 0.003 Gpa	Plastic strain 0.0
Fracture strength 0.005 Gpa	Plastic strain 0.25

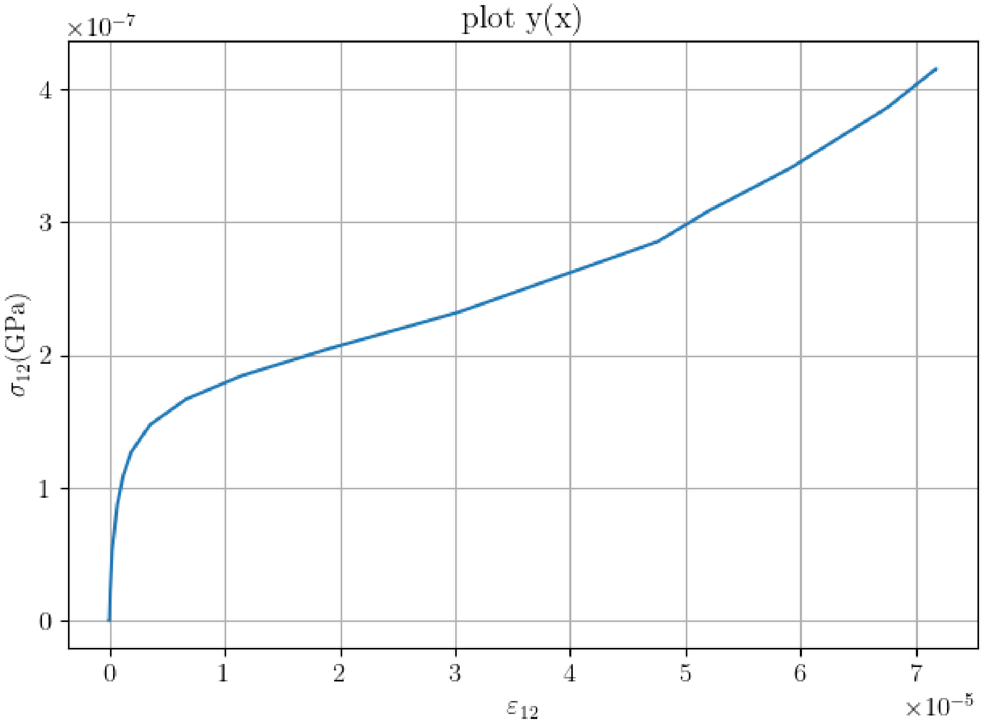
Young's modulus E = 1.0 Gpa	Poisson's ratio nu=0.3
Yield stress 0.002 Gpa	Plastic strain 0.0
Fracture strength 0.005 Gpa	Plastic strain 0.3

Flow curves of a micropillars compression $(20\mu m)$

Compression strength plot shows the linear hardening.

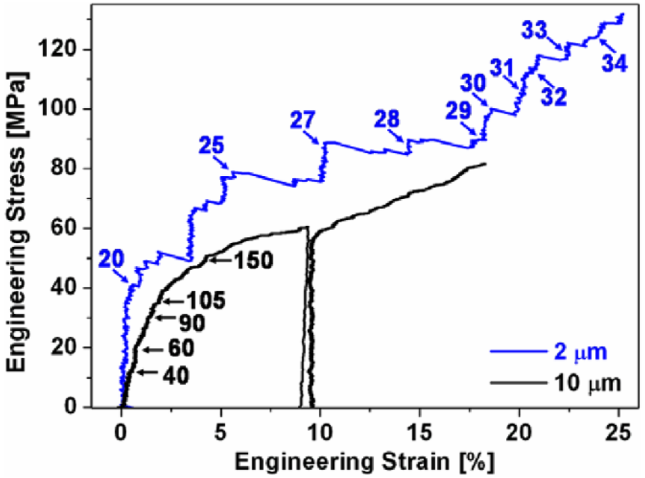


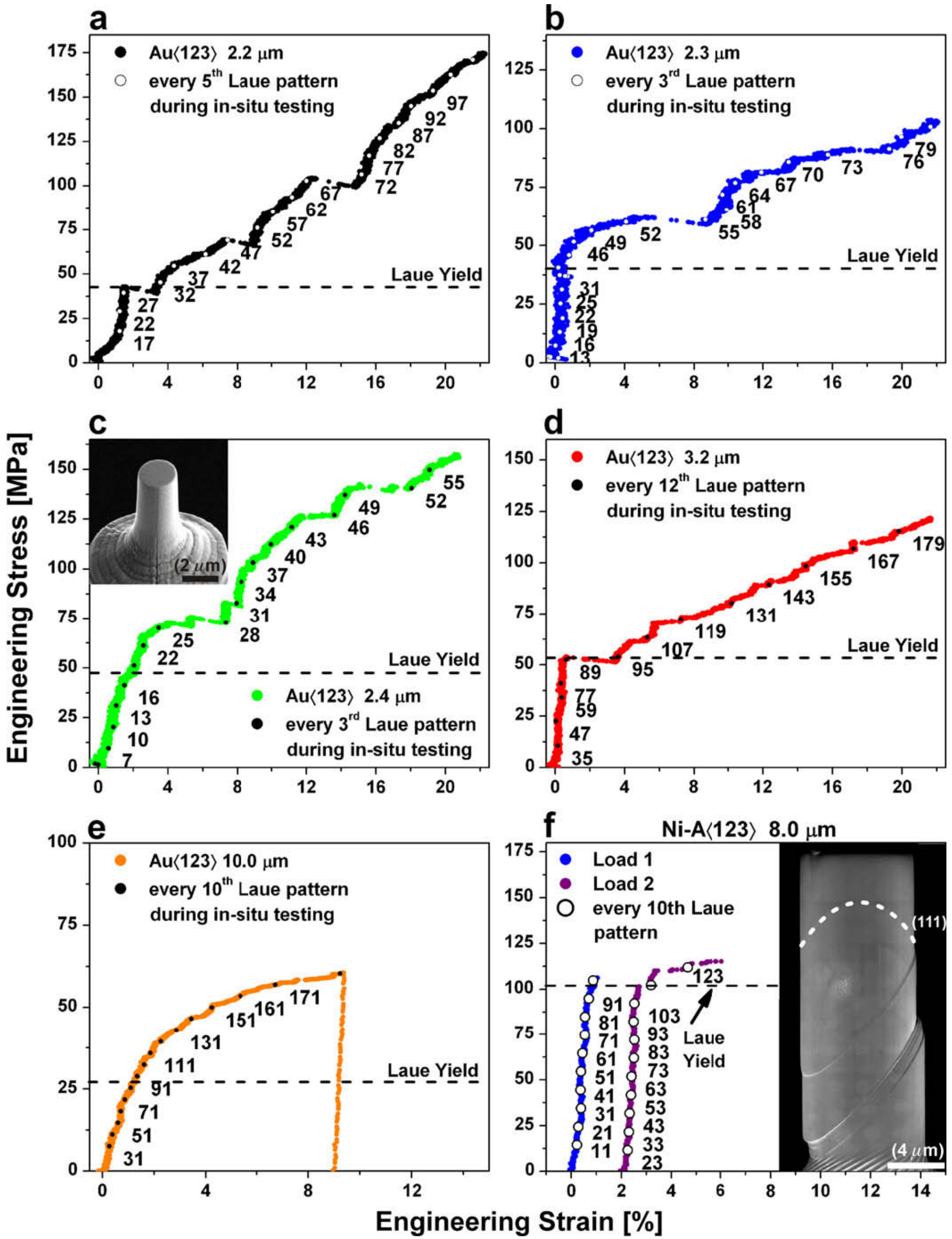
Shear strength plot shows the Frank-Read source.



Micropillar compression $(10\mu m)$

The strain-hardening behaves differently (smaller is stronger). The slip plane rotates for the strain compatibility.





Figures from Maaß et al. 2007 and 2009

Asaro's model

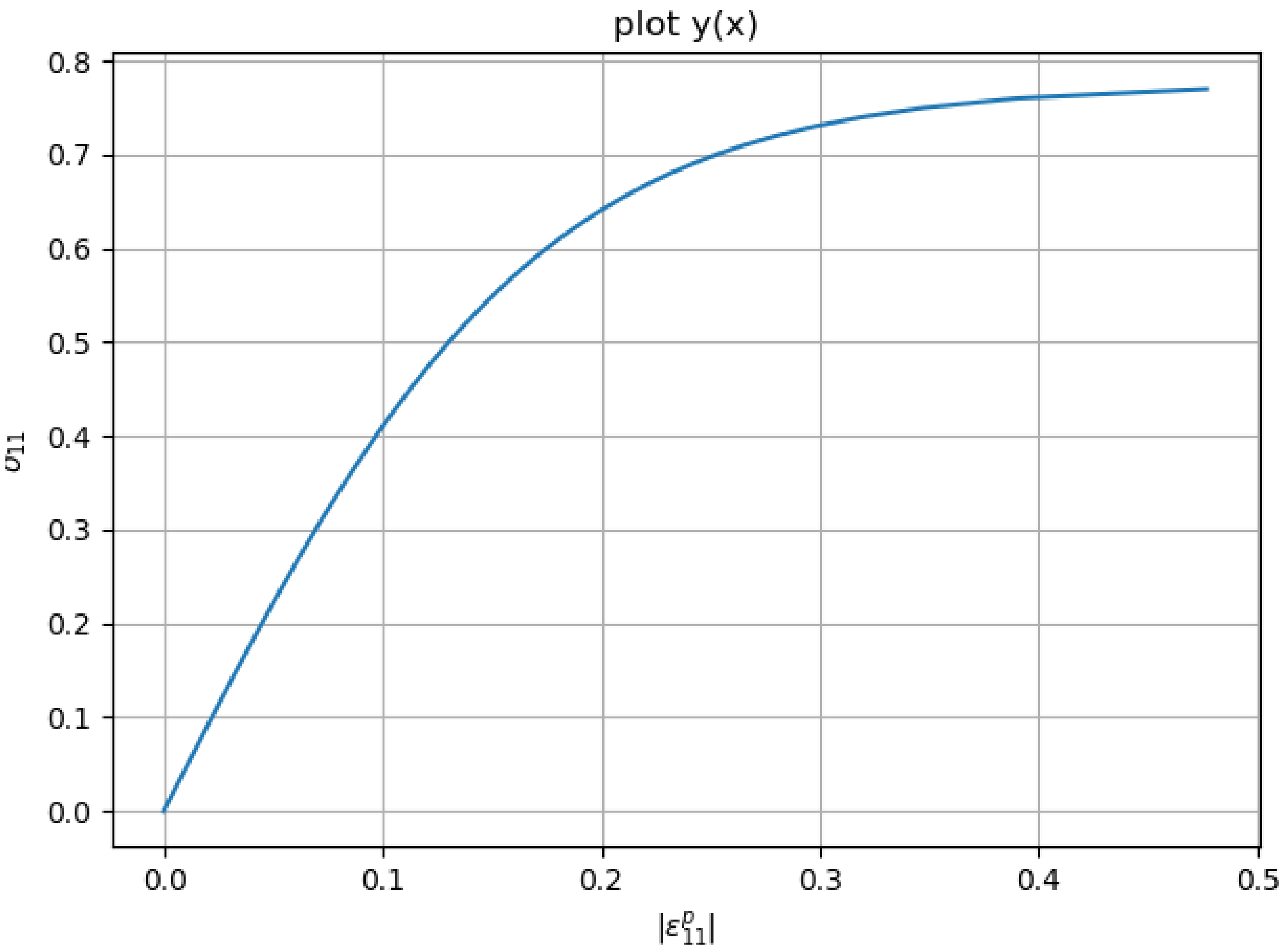
$h_{\alpha\alpha}(\gamma) = h_0 \operatorname{sech}^2 \left| \frac{h_0 \gamma}{\tau_s - \tau_0} \right|$ (no sum on α)

$h_{\alpha\beta}(\gamma) = q h_{\alpha\alpha}(\gamma)$ ($\alpha \neq \beta$)

$\gamma = \sum_\alpha \int_0^t |\dot{\gamma}^{(\alpha)}| \, dt$ is the Taylor cumulative shear strain on all slip systems.

The Asaro's model described the glide stage of work hardening.

h0	tau0	taus	q
1.0	1.0	2.0	1.4



Bassani-Wu model

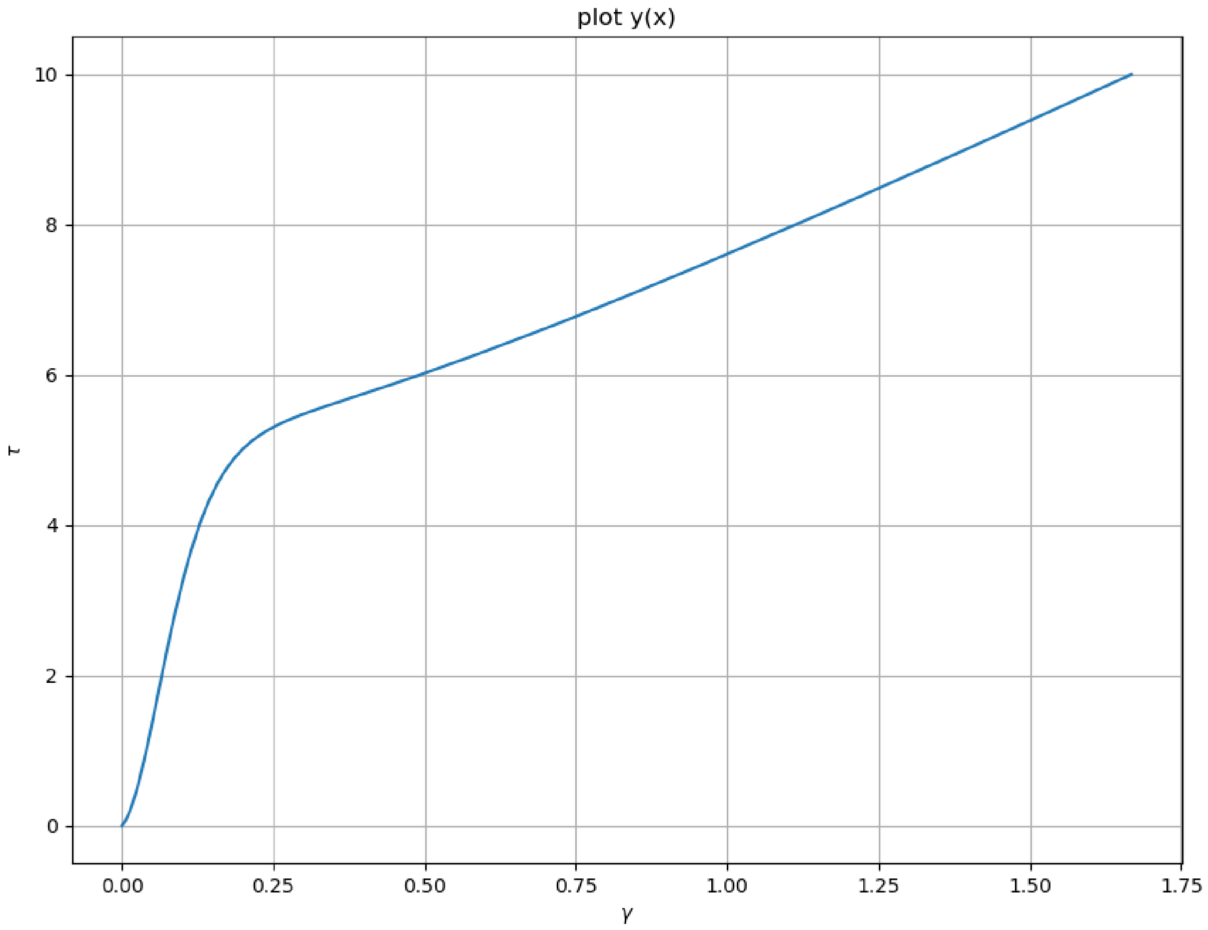
$h_{\alpha\alpha} = F(\gamma_\alpha) G\left(\{\gamma_\beta; \beta = 1, \dots N, \beta \neq \alpha\}\right)$ (no sum on α) ,

$h_{\beta\alpha} = q h_{\alpha\alpha}$, $\alpha \neq \beta$ (no sum on α) ,

$F(\gamma_\alpha) = \left\{(h_0 - h_s)\left(\operatorname{sech}\left[\frac{(h_0 - h_s)\gamma_\alpha}{\tau_s - \tau_0}\right]\right)^2 + h_s\right\}$,

$G\left(\{\gamma_\beta; \beta = 1, \dots N, \beta \neq \alpha\}\right) = 1 + \sum_{\beta=1,\beta\neq\alpha}^{N} f_{\alpha\beta} \tanh\left(\gamma_\beta / \gamma_0\right)$,

h0	tau0	taus	hs	q
1.0	1.0	2.0	0.01	1.4



Finite Strain

The deformation gradient is defined as

$$F = \frac{\partial x}{\partial X}$$

fulfills the property $J = \det(F) > 0$.

The deformation gradient in this definition has the polar decomposition

$$F = RU = VR$$

The Green deformation tensor is defined as

$$C = F^T F$$

and the Lagrangian strain is defined as

$$E = \frac{1}{2}(C - I)$$

The velocity gradient is defined as

$$L = \frac{\partial v}{\partial x} = \dot{F} F^{-1}$$

It has the symmetric part denoted deformation rate

$$D = \frac{1}{2}(L + L^T)$$

and skew-symmetric part denoted spin tensor

$$W = \frac{1}{2}(L - L^T)$$

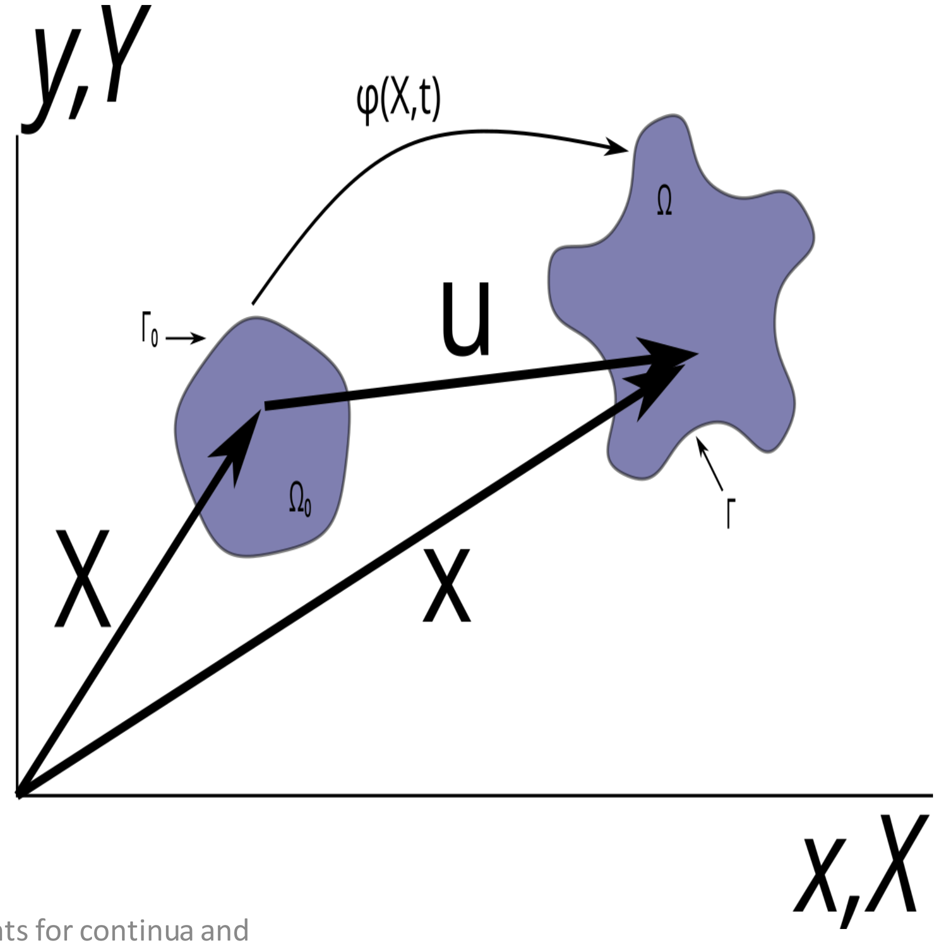


Figure from nonlinear finite elements for continua and structures, John Wiley & Sons, 2014

Lee’s decomposition

In order to model the material plastic properties, the deformation gradient can be decomposed as

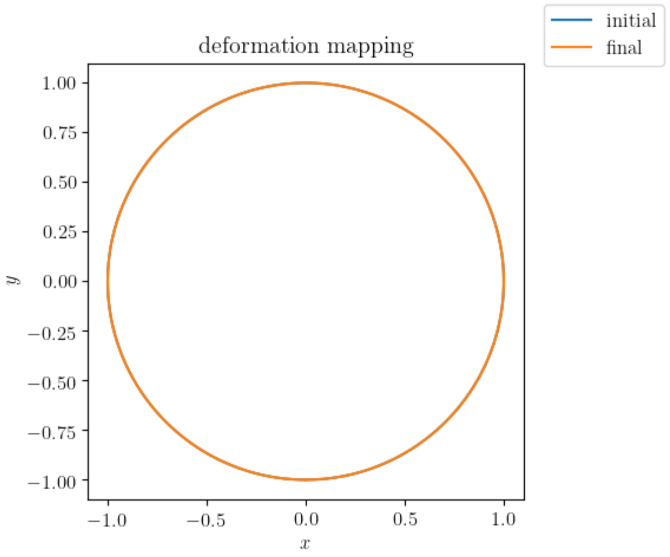
$$F = F^{el} F^{pl}$$

Inserting this formula into the velocity gradient,

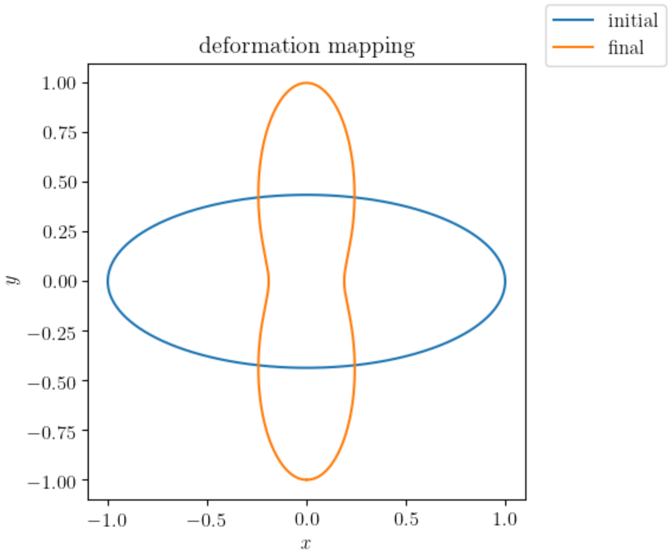
$$L = L^{el} + F^{el} L^{pl} \left(F^{el}\right)^{-1}$$

In such decomposition, the shear strain rate of the slip systems can be included,

$$L^{pl} = \sum_{\alpha=1}^{n} \dot{\gamma}^{\alpha} m^{\alpha} \otimes n^{\alpha}$$



F^{pl} is volume preserving.



F^{pl} is rotation exclusion.

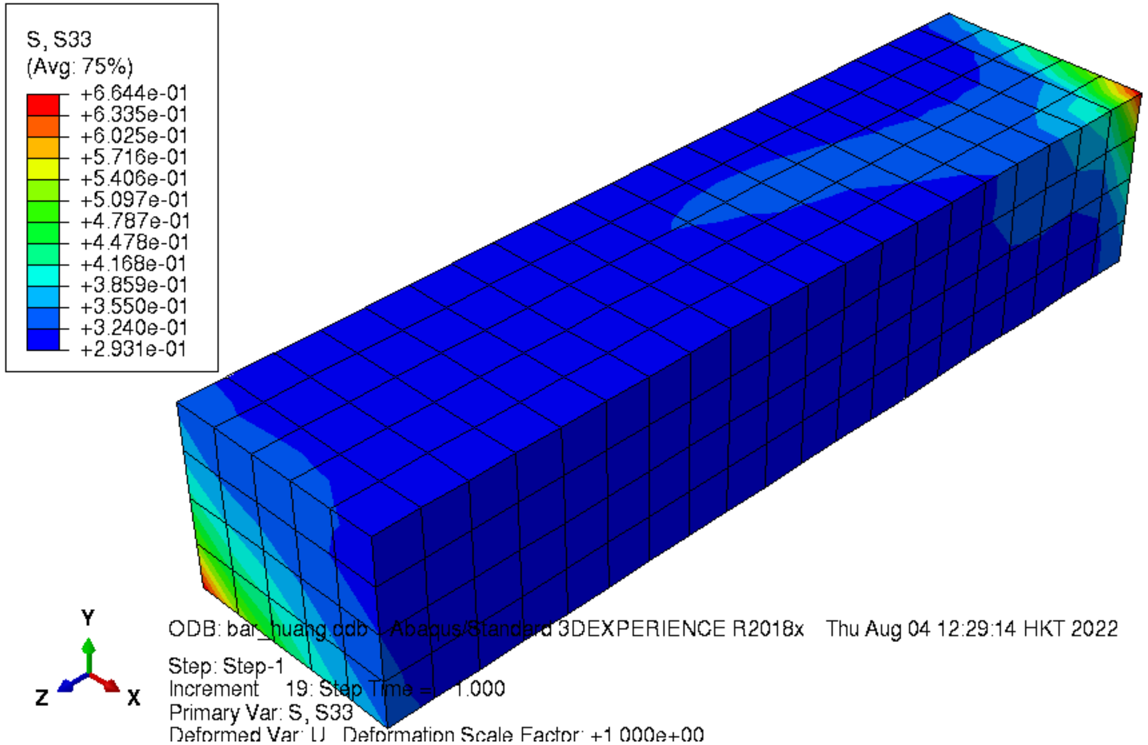
Viscoplastic power-law

The viscoplastic power-law relation is written in the following

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left(\frac{\tau^{\alpha}}{g^{\alpha}}\right)^{n}$$

where $\dot{\gamma}_0$ is a reference strain rate, n is the rate sensitivity exponent and g^{α} is the slip resistance of the αth system.

The Asaro's model and Bassani-Wu model can be embedded into the g^{α} term. In the simple cases (e.g. uniaxial tension), the material is rate-independent if the exponent is large, that is the smoothing of constitutive law. However, in the complex cases, the viscoplastic power-law is essential to find the stress concentration.



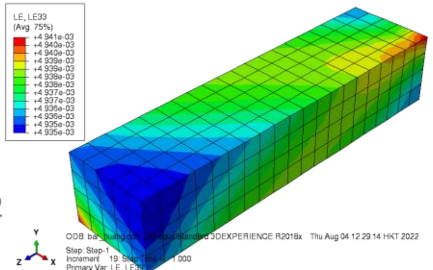
Huang's UMAT application

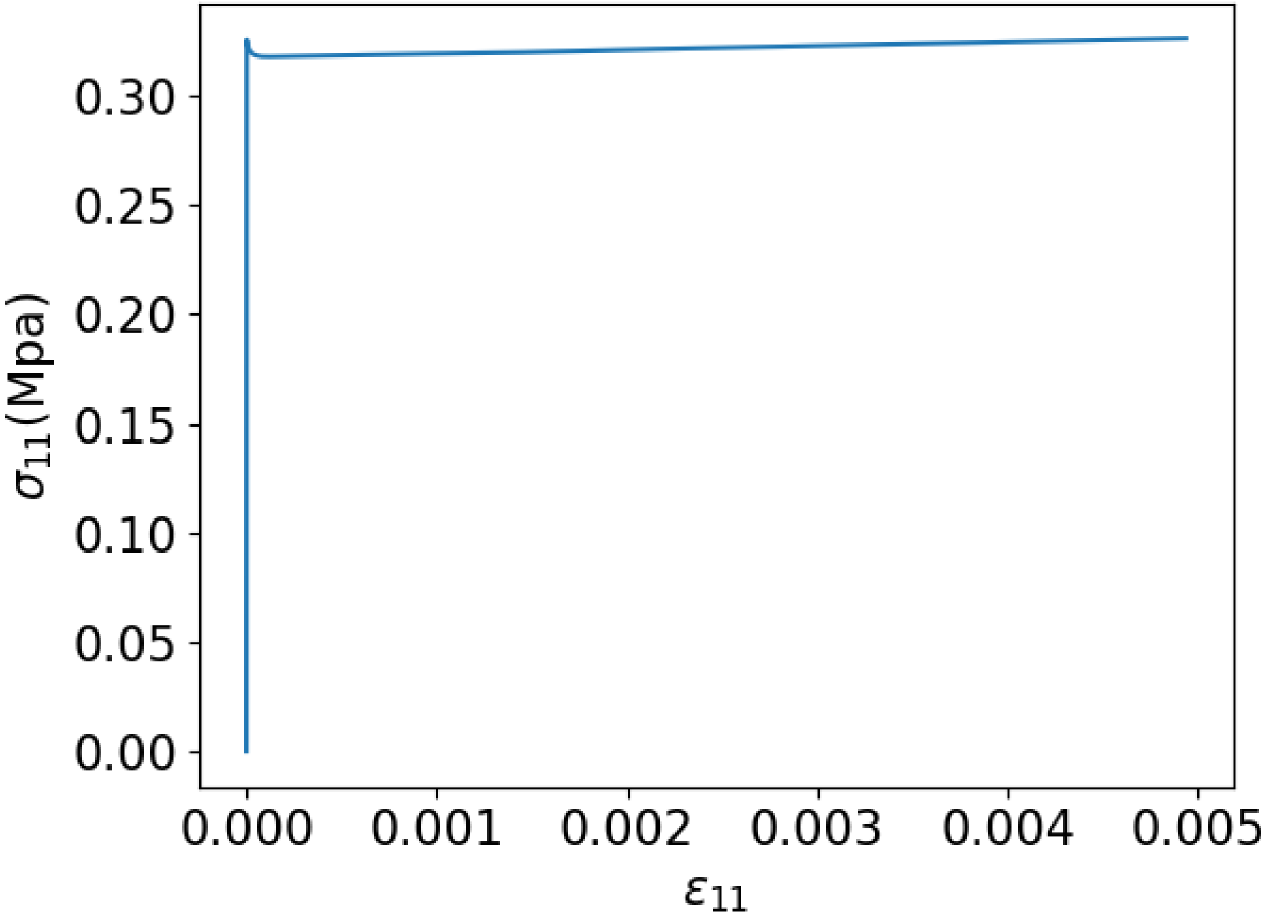
The parameters of Asaro's hardening law

C11(Mpa)	C12(Mpa)	C44(Mpa)
168400	121400	75400

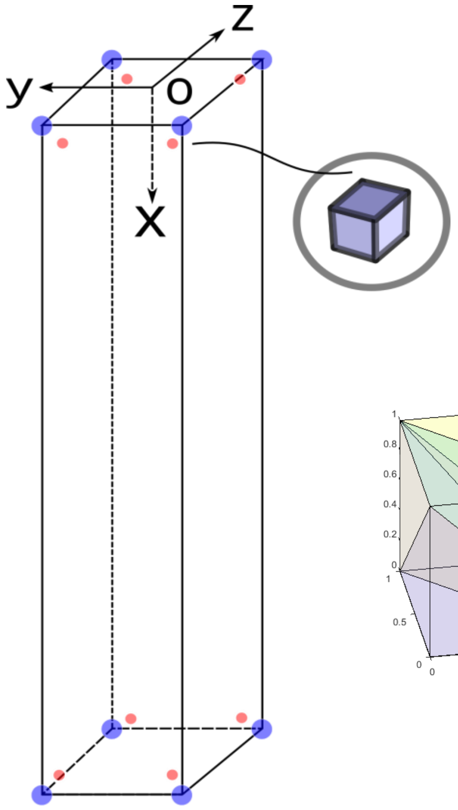
h0(Mpa)	taus(Mpa)	tau0(Mpa)
541.5	109.5	60.8

q	ql
1.0	1.4

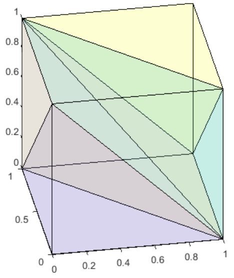




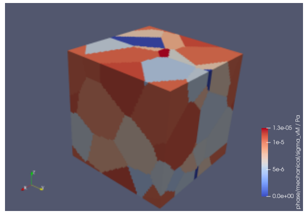
Representative Volume Element (RVE)



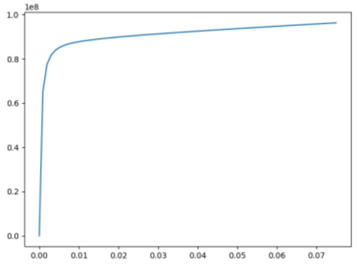
FEM

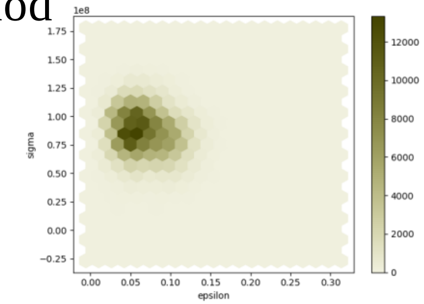


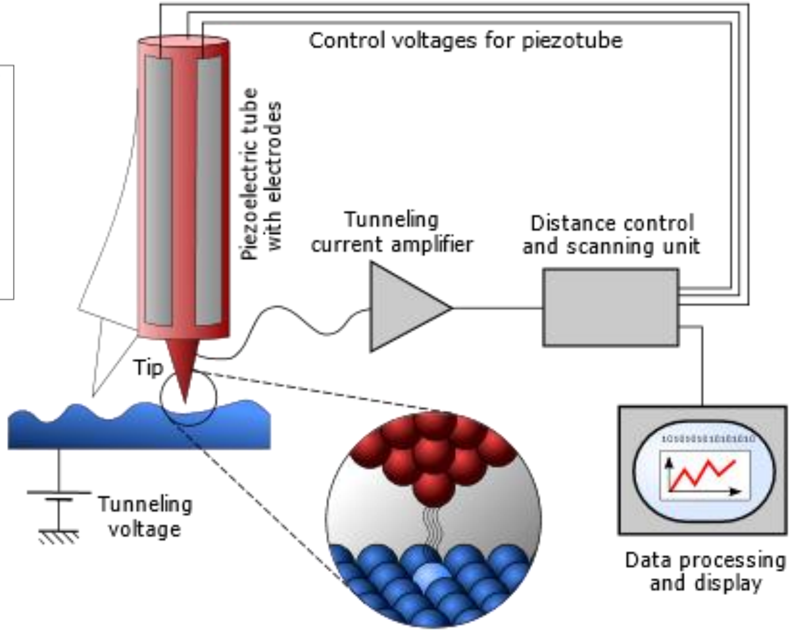
UMAT



Spectral method







Density functional theory

mm (10^{-3}m) μm (10^{-6}m) nm (10^{-9}m) Å (10^{-10}m)

See damask.mpie.de for details

End